# FIGURE 1

**Amino acid sequence for full-length E. coli IspA**

**[SEQ. ID No. 1]**

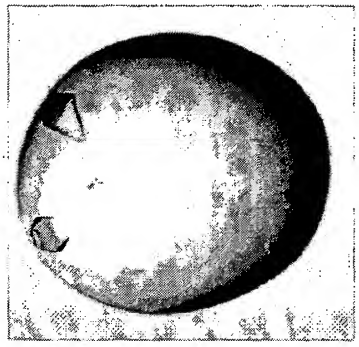
MGSDKIIHHHHHHTLMDFPQQLEACVKQANQALSRFIAPLPFQNTPVVETMQYGALLGGK
RLRPFLVYATGHMFGVSTNTLDAPAAAVECIHAYSLIHDDLPAMDDDDLRRGLPTCHVKF
GEANAILAGDALQTLAFSILSDADMPEVSDRDRISMISELASASGIAGMCGGQALDLDAE
GKHVPLDALERIHRHKTGALIRAAVRLGALSAGDKGRRALPVLDKYAESIGLAFQVQDDI
LDVVGDTATLGKRQGADQQLGKSTYPALLGLEQARKKARDLIDDARQSLKQLAEQSLDTS
ALEALADYIIQRNK

**cDNA sequence encoding IspA**

**[SEQ. ID No. 2]**

ATGGGATCTGATAAAATTATTCACCATCACCATCACCATACCCTTATGGACTTTCCGCAG
CAACTCGAAGCCTGCGTTAAGCAGGCCAACCAGGCGCTGAGCCGTTTTATCGCCCCACTG
CCCTTTCAGAACACTCCCGTGGTCGAAACCATGCAGTATGGCGCATTATTAGGTGGTAAG
CGCCTGCGACCTTTCCTGGTTTATGCCACCGGTCATATGTTCGGCGTTAGCACAAACACG
CTGGACGCACCCGCTGCCGCCGTTGAGTGTATCCACGCTTACTCATTAATTCATGATGAT
TTACCGGCAATGGATGATGACGATCTGCGTCGCGGTTTGCCAACCTGCCATGTGAAGTTT
GGCGAAGCAAACGCGATTCTCGCTGGCGACGCTTTACAAACGCTGGCGTTCTCGATTTTA
AGCGATGCCGATATGCCGGAAGTGTCGGACCGCGACAGAATTTCGATGATTTCTGAACTG
GCGAGCGCCAGTGGTATTGCCGGAATGTGCGGTGGTCAGGCATTAGATTTAGACGCGGAA
GGCAAACACGTACCTCTGGACGCGCTTGAGCGTATTCATCGTCATAAAACCGGCGCATTG
ATTCGCGCCGCCGTTCGCCTTGGTGCATTAAGCGCCGGAGATAAAGGACGTCGTGCTCTG
CCGGTACTCGACAAGTATGCAGAGAGCATCGGCCTTGCCTTCCAGGTTCAGGATGACATC
CTGGATGTGGTGGGAGATACTGCAACGTTGGGAAAACGCCAGGGTGCCGACCAGCAACTT
GGTAAAAGTACCTACCCTGCACTTCTGGGTCTTGAGCAAGCCCGGAAGAAAGCCCGGGAT
CTGATCGACGATGCCCGTCAGTCGCTGAAACAACTGGCTGAACAGTCACTCGATACCTCG
GCACTGGAAGCGCTAGCGGACTACATCATCCAGCGTAATAAATAA

# FIGURE 2



# FIGURE 3

## LEGEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number', (F)'X Coordinate', (G)'Y Coordinate', (H)'Z Coordinate', (I)'Occupancy' (OCC) and (J)'B factor'.

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 1 | N | MET | A | 22 | 65.564 | 50.628 | -5.933 | 1.00 | 45.23 |
| 3 | CA | MET | A | 22 | 65.166 | 51.178 | -7.255 | 1.00 | 44.87 |
| 5 | CB | MET | A | 22 | 64.933 | 50.049 | -8.267 | 1.00 | 45.30 |
| 8 | CG | MET | A | 22 | 65.153 | 50.446 | -9.726 | 1.00 | 47.01 |
| 11 | SD | MET | A | 22 | 66.181 | 49.252 | -10.631 | 1.00 | 50.95 |
| 12 | CE | MET | A | 22 | 64.933 | 48.059 | -11.220 | 1.00 | 50.52 |
| 16 | C | MET | A | 22 | 63.907 | 52.030 | -7.120 | 1.00 | 43.94 |
| 17 | O | MET | A | 22 | 63.880 | 53.159 | -7.610 | 1.00 | 44.23 |
| 20 | N | ASP | A | 23 | 62.875 | 51.491 | -6.466 | 1.00 | 42.41 |
| 22 | CA | ASP | A | 23 | 61.591 | 52.188 | -6.366 | 1.00 | 41.35 |
| 24 | CB | ASP | A | 23 | 60.409 | 51.226 | -6.459 | 1.00 | 41.74 |
| 27 | CG | ASP | A | 23 | 59.134 | 51.926 | -6.899 | 1.00 | 43.33 |
| 28 | OD1 | ASP | A | 23 | 58.448 | 52.535 | -6.037 | 1.00 | 46.33 |
| 29 | OD2 | ASP | A | 23 | 58.753 | 51.939 | -8.093 | 1.00 | 45.52 |
| 30 | C | ASP | A | 23 | 61.486 | 52.990 | -5.079 | 1.00 | 39.80 |
| 31 | O | ASP | A | 23 | 61.195 | 52.441 | -4.005 | 1.00 | 38.54 |
| 32 | N | PHE | A | 24 | 61.672 | 54.298 | -5.210 | 1.00 | 38.05 |
| 34 | CA | PHE | A | 24 | 61.858 | 55.146 | -4.050 | 1.00 | 36.90 |
| 36 | CB | PHE | A | 24 | 62.429 | 56.514 | -4.427 | 1.00 | 36.92 |
| 39 | CG | PHE | A | 24 | 63.016 | 57.233 | -3.260 | 1.00 | 36.41 |
| 40 | CD1 | PHE | A | 24 | 64.116 | 56.707 | -2.609 | 1.00 | 37.05 |
| 42 | CE1 | PHE | A | 24 | 64.658 | 57.340 | -1.502 | 1.00 | 36.55 |
| 44 | CZ | PHE | A | 24 | 64.098 | 58.493 | -1.036 | 1.00 | 36.07 |
| 46 | CE2 | PHE | A | 24 | 62.988 | 59.025 | -1.664 | 1.00 | 36.56 |
| 48 | CD2 | PHE | A | 24 | 62.442 | 58.392 | -2.768 | 1.00 | 36.65 |
| 50 | C | PHE | A | 24 | 60.632 | 55.314 | -3.158 | 1.00 | 35.80 |
| 51 | O | PHE | A | 24 | 60.769 | 55.198 | -1.949 | 1.00 | 35.17 |
| 52 | N | PRO | A | 25 | 59.456 | 55.618 | -3.712 | 1.00 | 34.90 |
| 53 | CA | PRO | A | 25 | 58.239 | 55.676 | -2.889 | 1.00 | 34.06 |
| 55 | CB | PRO | A | 25 | 57.123 | 55.861 | -3.924 | 1.00 | 34.29 |
| 58 | CG | PRO | A | 25 | 57.782 | 56.558 | -5.047 | 1.00 | 34.27 |
| 61 | CD | PRO | A | 25 | 59.176 | 55.993 | -5.114 | 1.00 | 34.77 |
| 64 | C | PRO | A | 25 | 58.008 | 54.418 | -2.039 | 1.00 | 33.38 |
| 65 | O | PRO | A | 25 | 57.585 | 54.564 | -0.895 | 1.00 | 32.65 |
| 66 | N | GLN | A | 26 | 58.279 | 53.228 | -2.579 | 1.00 | 32.48 |
| 68 | CA | GLN | A | 26 | 58.126 | 51.981 | -1.815 | 1.00 | 32.23 |
| 70 | CB | GLN | A | 26 | 58.188 | 50.746 | -2.732 | 1.00 | 32.68 |
| 73 | CG | GLN | A | 26 | 56.883 | 50.493 | -3.534 | 1.00 | 35.01 |
| 76 | CD | GLN | A | 26 | 56.611 | 49.011 | -3.811 | 1.00 | 39.06 |
| 77 | OE1 | GLN | A | 26 | 55.463 | 48.546 | -3.685 | 1.00 | 41.57 |
| 78 | NE2 | GLN | A | 26 | 57.654 | 48.270 | -4.193 | 1.00 | 39.95 |
| 81 | C | GLN | A | 26 | 59.177 | 51.869 | -0.700 | 1.00 | 30.90 |
| 82 | O | GLN | A | 26 | 58.892 | 51.363 | 0.379 | 1.00 | 30.03 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 83 | N | GLN | A | 27 | 60.385 | 52.351 | -0.959 | 1.00 | 29.82 |
| 85 | CA | GLN | A | 27 | 61.426 | 52.370 | 0.058 | 1.00 | 29.68 |
| 87 | CB | GLN | A | 27 | 62.783 | 52.738 | -0.560 | 1.00 | 29.82 |
| 90 | CG | GLN | A | 27 | 63.366 | 51.647 | -1.494 | 1.00 | 31.98 |
| 93 | CD | GLN | A | 27 | 63.920 | 50.425 | -0.746 | 1.00 | 34.89 |
| 94 | OE1 | GLN | A | 27 | 64.483 | 49.512 | -1.360 | 1.00 | 36.76 |
| 95 | NE2 | GLN | A | 27 | 63.762 | 50.412 | 0.572 | 1.00 | 37.29 |
| 98 | C | GLN | A | 27 | 61.065 | 53.323 | 1.204 | 1.00 | 28.61 |
| 99 | O | GLN | A | 27 | 61.214 | 52.973 | 2.372 | 1.00 | 28.03 |
| 100 | N | LEU | A | 28 | 60.588 | 54.513 | 0.863 | 1.00 | 27.80 |
| 102 | CA | LEU | A | 28 | 60.120 | 55.472 | 1.848 | 1.00 | 27.76 |
| 104 | CB | LEU | A | 28 | 59.582 | 56.740 | 1.169 | 1.00 | 28.15 |
| 107 | CG | LEU | A | 28 | 60.595 | 57.714 | 0.543 | 1.00 | 29.56 |
| 109 | CD1 | LEU | A | 28 | 59.880 | 58.764 | -0.297 | 1.00 | 30.48 |
| 113 | CD2 | LEU | A | 28 | 61.447 | 58.392 | 1.611 | 1.00 | 30.42 |
| 117 | C | LEU | A | 28 | 59.036 | 54.861 | 2.736 | 1.00 | 27.31 |
| 118 | O | LEU | A | 28 | 59.099 | 54.975 | 3.950 | 1.00 | 26.43 |
| 119 | N | GLU | A | 29 | 58.057 | 54.185 | 2.145 | 1.00 | 27.14 |
| 121 | CA | GLU | A | 29 | 56.973 | 53.627 | 2.952 | 1.00 | 27.44 |
| 123 | CB | GLU | A | 29 | 55.760 | 53.232 | 2.101 | 1.00 | 28.34 |
| 126 | CG | GLU | A | 29 | 54.798 | 52.234 | 2.759 | 1.00 | 31.44 |
| 129 | CD | GLU | A | 29 | 53.961 | 52.789 | 3.912 | 1.00 | 35.82 |
| 130 | OE1 | GLU | A | 29 | 52.791 | 52.370 | 4.024 | 1.00 | 38.87 |
| 131 | OE2 | GLU | A | 29 | 54.448 | 53.597 | 4.738 | 1.00 | 38.87 |
| 132 | C | GLU | A | 29 | 57.465 | 52.462 | 3.805 | 1.00 | 26.15 |
| 133 | O | GLU | A | 29 | 57.040 | 52.322 | 4.949 | 1.00 | 25.29 |
| 134 | N | ALA | A | 30 | 58.357 | 51.642 | 3.254 | 1.00 | 25.31 |
| 136 | CA | ALA | A | 30 | 59.018 | 50.578 | 4.013 | 1.00 | 24.72 |
| 138 | CB | ALA | A | 30 | 60.019 | 49.847 | 3.153 | 1.00 | 25.46 |
| 142 | C | ALA | A | 30 | 59.728 | 51.160 | 5.230 | 1.00 | 24.33 |
| 143 | O | ALA | A | 30 | 59.610 | 50.636 | 6.331 | 1.00 | 23.33 |
| 144 | N | CYS | A | 31 | 60.438 | 52.263 | 5.025 | 1.00 | 23.38 |
| 146 | CA | CYS | A | 31 | 61.130 | 52.944 | 6.115 | 1.00 | 23.00 |
| 148 | CB | CYS | A | 31 | 62.029 | 54.056 | 5.578 | 1.00 | 23.11 |
| 151 | SG | CYS | A | 31 | 62.861 | 54.980 | 6.885 | 1.00 | 21.11 |
| 152 | C | CYS | A | 31 | 60.147 | 53.499 | 7.162 | 1.00 | 22.39 |
| 153 | O | CYS | A | 31 | 60.368 | 53.344 | 8.351 | 1.00 | 22.44 |
| 154 | N | VAL | A | 32 | 59.051 | 54.105 | 6.725 | 1.00 | 22.24 |
| 156 | CA | VAL | A | 32 | 58.056 | 54.638 | 7.651 | 1.00 | 22.18 |
| 158 | CB | VAL | A | 32 | 56.889 | 55.349 | 6.902 | 1.00 | 22.57 |
| 160 | CG1 | VAL | A | 32 | 55.697 | 55.610 | 7.815 | 1.00 | 22.85 |
| 164 | CG2 | VAL | A | 32 | 57.368 | 56.650 | 6.293 | 1.00 | 22.19 |
| 168 | C | VAL | A | 32 | 57.534 | 53.530 | 8.580 | 1.00 | 21.91 |
| 169 | O | VAL | A | 32 | 57.440 | 53.722 | 9.789 | 1.00 | 21.65 |
| 170 | N | LYS | A | 33 | 57.235 | 52.369 | 8.011 | 1.00 | 21.41 |
| 172 | CA | LYS | A | 33 | 56.741 | 51.236 | 8.779 | 1.00 | 21.24 |
| 174 | CB | LYS | A | 33 | 56.273 | 50.127 | 7.836 | 1.00 | 22.15 |
| 177 | CG | LYS | A | 33 | 54.982 | 50.454 | 7.081 | 1.00 | 24.03 |
| 180 | CD | LYS | A | 33 | 54.467 | 49.210 | 6.340 | 1.00 | 28.62 |
| 183 | CE | LYS | A | 33 | 53.133 | 49.458 | 5.596 | 1.00 | 31.91 |
| 186 | NZ | LYS | A | 33 | 53.166 | 48.924 | 4.184 | 1.00 | 33.67 |
| 190 | C | LYS | A | 33 | 57.798 | 50.693 | 9.737 | 1.00 | 20.33 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 191 | O | LYS | A | 33 | 57.499 | 50.428 | 10.910 | 1.00 | 19.84 |
| 192 | N | GLN | A | 34 | 59.022 | 50.536 | 9.244 | 1.00 | 19.37 |
| 194 | CA | GLN | A | 34 | 60.116 | 50.039 | 10.073 | 1.00 | 19.22 |
| 196 | CB | GLN | A | 34 | 61.413 | 49.892 | 9.264 | 1.00 | 19.05 |
| 199 | CG | GLN | A | 34 | 62.596 | 49.326 | 10.078 | 1.00 | 19.21 |
| 202 | CD | GLN | A | 34 | 62.485 | 47.814 | 10.392 | 1.00 | 20.65 |
| 203 | OE1 | GLN | A | 34 | 63.076 | 47.320 | 11.375 | 1.00 | 22.34 |
| 204 | NE2 | GLN | A | 34 | 61.792 | 47.087 | 9.537 | 1.00 | 16.09 |
| 207 | C | GLN | A | 34 | 60.340 | 50.985 | 11.258 | 1.00 | 18.67 |
| 208 | O | GLN | A | 34 | 60.392 | 50.549 | 12.386 | 1.00 | 18.19 |
| 209 | N | ALA | A | 35 | 60.465 | 52.278 | 10.985 | 1.00 | 18.55 |
| 211 | CA | ALA | A | 35 | 60.748 | 53.271 | 12.026 | 1.00 | 18.70 |
| 213 | CB | ALA | A | 35 | 61.022 | 54.625 | 11.403 | 1.00 | 18.98 |
| 217 | C | ALA | A | 35 | 59.626 | 53.382 | 13.036 | 1.00 | 19.64 |
| 218 | O | ALA | A | 35 | 59.875 | 53.535 | 14.238 | 1.00 | 19.64 |
| 219 | N | ASN | A | 36 | 58.386 | 53.300 | 12.564 | 1.00 | 19.52 |
| 221 | CA | ASN | A | 36 | 57.232 | 53.369 | 13.464 | 1.00 | 19.96 |
| 223 | CB | ASN | A | 36 | 55.920 | 53.446 | 12.688 | 1.00 | 19.83 |
| 226 | CG | ASN | A | 36 | 55.652 | 54.816 | 12.118 | 1.00 | 22.13 |
| 227 | OD1 | ASN | A | 36 | 56.322 | 55.792 | 12.458 | 1.00 | 23.82 |
| 228 | ND2 | ASN | A | 36 | 54.638 | 54.904 | 11.249 | 1.00 | 23.36 |
| 231 | C | ASN | A | 36 | 57.177 | 52.190 | 14.405 | 1.00 | 19.86 |
| 232 | O | ASN | A | 36 | 56.847 | 52.343 | 15.573 | 1.00 | 19.83 |
| 233 | N | GLN | A | 37 | 57.474 | 51.010 | 13.878 | 1.00 | 20.51 |
| 235 | CA | GLN | A | 37 | 57.584 | 49.779 | 14.679 | 1.00 | 21.34 |
| 237 | CB | GLN | A | 37 | 57.921 | 48.608 | 13.760 | 1.00 | 21.77 |
| 240 | CG | GLN | A | 37 | 57.882 | 47.246 | 14.412 | 1.00 | 24.92 |
| 243 | CD | GLN | A | 37 | 58.025 | 46.137 | 13.385 | 1.00 | 29.08 |
| 244 | OE1 | GLN | A | 37 | 59.120 | 45.918 | 12.832 | 1.00 | 33.06 |
| 245 | NE2 | GLN | A | 37 | 56.929 | 45.446 | 13.112 | 1.00 | 31.52 |
| 248 | C | GLN | A | 37 | 58.683 | 49.902 | 15.737 | 1.00 | 21.05 |
| 249 | O | GLN | A | 37 | 58.488 | 49.550 | 16.899 | 1.00 | 20.55 |
| 250 | N | ALA | A | 38 | 59.839 | 50.384 | 15.310 | 1.00 | 20.90 |
| 252 | CA | ALA | A | 38 | 60.957 | 50.629 | 16.213 | 1.00 | 21.59 |
| 254 | CB | ALA | A | 38 | 62.129 | 51.176 | 15.451 | 1.00 | 21.36 |
| 258 | C | ALA | A | 38 | 60.539 | 51.598 | 17.315 | 1.00 | 21.65 |
| 259 | O | ALA | A | 38 | 60.696 | 51.304 | 18.475 | 1.00 | 22.05 |
| 260 | N | LEU | A | 39 | 59.999 | 52.750 | 16.940 | 1.00 | 22.61 |
| 262 | CA | LEU | A | 39 | 59.575 | 53.760 | 17.906 | 1.00 | 23.19 |
| 264 | CB | LEU | A | 39 | 58.931 | 54.937 | 17.175 | 1.00 | 23.47 |
| 267 | CG | LEU | A | 39 | 59.879 | 55.966 | 16.574 | 1.00 | 24.21 |
| 269 | CD1 | LEU | A | 39 | 59.165 | 56.759 | 15.502 | 1.00 | 24.68 |
| 273 | CD2 | LEU | A | 39 | 60.391 | 56.887 | 17.685 | 1.00 | 26.09 |
| 277 | C | LEU | A | 39 | 58.555 | 53.183 | 18.890 | 1.00 | 24.35 |
| 278 | O | LEU | A | 39 | 58.659 | 53.391 | 20.094 | 1.00 | 23.66 |
| 279 | N | SER | A | 40 | 57.567 | 52.471 | 18.356 | 1.00 | 25.27 |
| 281 | CA | SER | A | 40 | 56.513 | 51.879 | 19.172 | 1.00 | 26.76 |
| 283 | CB | SER | A | 40 | 55.480 | 51.162 | 18.295 | 1.00 | 27.01 |
| 286 | OG | SER | A | 40 | 54.789 | 52.077 | 17.470 | 1.00 | 28.06 |
| 288 | C | SER | A | 40 | 57.070 | 50.896 | 20.194 | 1.00 | 27.73 |
| 289 | O | SER | A | 40 | 56.597 | 50.849 | 21.316 | 1.00 | 28.77 |
| 290 | N | ARG | A | 41 | 58.071 | 50.117 | 19.802 | 1.00 | 28.38 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 292 | CA | ARG | A | 41 | 58.649 | 49.117 | 20.688 | 1.00 | 29.15 |
| 294 | CB | ARG | A | 41 | 59.580 | 48.182 | 19.915 | 1.00 | 29.68 |
| 297 | CG | ARG | A | 41 | 58.842 | 47.176 | 19.053 | 1.00 | 33.37 |
| 300 | CD | ARG | A | 41 | 59.681 | 46.648 | 17.895 | 1.00 | 36.27 |
| 303 | NE | ARG | A | 41 | 59.113 | 45.445 | 17.291 | 1.00 | 39.06 |
| 305 | CZ | ARG | A | 41 | 59.778 | 44.630 | 16.473 | 1.00 | 41.04 |
| 306 | NH1 | ARG | A | 41 | 61.046 | 44.878 | 16.153 | 1.00 | 42.52 |
| 309 | NH2 | ARG | A | 41 | 59.174 | 43.564 | 15.970 | 1.00 | 42.39 |
| 312 | C | ARG | A | 41 | 59.426 | 49.761 | 21.828 | 1.00 | 28.40 |
| 313 | O | ARG | A | 41 | 59.480 | 49.210 | 22.926 | 1.00 | 27.74 |
| 314 | N | PHE | A | 42 | 60.045 | 50.910 | 21.557 | 1.00 | 27.61 |
| 316 | CA | PHE | A | 42 | 60.785 | 51.634 | 22.587 | 1.00 | 27.39 |
| 318 | CB | PHE | A | 42 | 61.853 | 52.533 | 21.960 | 1.00 | 27.18 |
| 321 | CG | PHE | A | 42 | 62.924 | 51.766 | 21.240 | 1.00 | 25.69 |
| 322 | CD1 | PHE | A | 42 | 63.214 | 52.029 | 19.918 | 1.00 | 25.01 |
| 324 | CE1 | PHE | A | 42 | 64.194 | 51.311 | 19.253 | 1.00 | 25.43 |
| 326 | CZ | PHE | A | 42 | 64.881 | 50.295 | 19.910 | 1.00 | 26.41 |
| 328 | CE2 | PHE | A | 42 | 64.600 | 50.022 | 21.218 | 1.00 | 26.08 |
| 330 | CD2 | PHE | A | 42 | 63.624 | 50.755 | 21.886 | 1.00 | 25.98 |
| 332 | C | PHE | A | 42 | 59.855 | 52.427 | 23.491 | 1.00 | 27.72 |
| 333 | O | PHE | A | 42 | 60.189 | 52.684 | 24.642 | 1.00 | 27.44 |
| 334 | N | ILE | A | 43 | 58.679 | 52.775 | 22.979 | 1.00 | 27.76 |
| 336 | CA | ILE | A | 43 | 57.677 | 53.488 | 23.756 | 1.00 | 28.44 |
| 338 | CB | ILE | A | 43 | 56.779 | 54.342 | 22.815 | 1.00 | 28.50 |
| 340 | CG1 | ILE | A | 43 | 57.527 | 55.620 | 22.419 | 1.00 | 28.68 |
| 343 | CD1 | ILE | A | 43 | 56.932 | 56.377 | 21.266 | 1.00 | 29.67 |
| 347 | CG2 | ILE | A | 43 | 55.440 | 54.687 | 23.473 | 1.00 | 29.47 |
| 351 | C | ILE | A | 43 | 56.831 | 52.526 | 24.620 | 1.00 | 28.85 |
| 352 | O | ILE | A | 43 | 56.394 | 52.900 | 25.707 | 1.00 | 29.06 |
| 353 | N | ALA | A | 44 | 56.631 | 51.293 | 24.156 | 1.00 | 29.01 |
| 355 | CA | ALA | A | 44 | 55.688 | 50.357 | 24.797 | 1.00 | 29.51 |
| 357 | CB | ALA | A | 44 | 55.489 | 49.108 | 23.926 | 1.00 | 29.54 |
| 361 | C | ALA | A | 44 | 55.995 | 49.951 | 26.251 | 1.00 | 29.76 |
| 362 | O | ALA | A | 44 | 55.058 | 49.805 | 27.032 | 1.00 | 30.41 |
| 363 | N | PRO | A | 45 | 57.261 | 49.761 | 26.631 | 1.00 | 29.96 |
| 364 | CA | PRO | A | 45 | 57.590 | 49.430 | 28.028 | 1.00 | 29.81 |
| 366 | CB | PRO | A | 45 | 59.019 | 48.871 | 27.952 | 1.00 | 29.63 |
| 369 | CG | PRO | A | 45 | 59.465 | 48.986 | 26.511 | 1.00 | 30.25 |
| 372 | CD | PRO | A | 45 | 58.466 | 49.813 | 25.784 | 1.00 | 30.23 |
| 375 | C | PRO | A | 45 | 57.547 | 50.605 | 29.003 | 1.00 | 29.35 |
| 376 | O | PRO | A | 45 | 57.768 | 50.409 | 30.200 | 1.00 | 29.40 |
| 377 | N | LEU | A | 46 | 57.288 | 51.808 | 28.508 | 1.00 | 28.66 |
| 379 | CA | LEU | A | 46 | 57.243 | 52.978 | 29.364 | 1.00 | 27.78 |
| 381 | CB | LEU | A | 46 | 57.200 | 54.260 | 28.535 | 1.00 | 27.92 |
| 384 | CG | LEU | A | 46 | 58.410 | 54.574 | 27.654 | 1.00 | 28.42 |
| 386 | CD1 | LEU | A | 46 | 58.185 | 55.906 | 26.946 | 1.00 | 29.06 |
| 390 | CD2 | LEU | A | 46 | 59.716 | 54.573 | 28.481 | 1.00 | 28.93 |
| 394 | C | LEU | A | 46 | 56.009 | 52.911 | 30.243 | 1.00 | 27.39 |
| 395 | O | LEU | A | 46 | 54.962 | 52.410 | 29.814 | 1.00 | 27.10 |
| 396 | N | PRO | A | 47 | 56.115 | 53.412 | 31.471 | 1.00 | 26.65 |
| 397 | CA | PRO | A | 47 | 54.937 | 53.506 | 32.338 | 1.00 | 26.24 |
| 399 | CB | PRO | A | 47 | 55.528 | 53.818 | 33.719 | 1.00 | 26.42 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 402 | CG | PRO | A | 47 | 56.887 | 54.444 | 33.440 | 1.00 | 26.56 |
| 405 | CD | PRO | A | 47 | 57.339 | 53.909 | 32.122 | 1.00 | 26.41 |
| 408 | C | PRO | A | 47 | 54.017 | 54.624 | 31.863 | 1.00 | 25.76 |
| 409 | O | PRO | A | 47 | 54.386 | 55.397 | 30.977 | 1.00 | 25.20 |
| 410 | N | PHE | A | 48 | 52.840 | 54.706 | 32.469 | 1.00 | 25.70 |
| 412 | CA | PHE | A | 48 | 51.873 | 55.765 | 32.212 | 1.00 | 25.79 |
| 414 | CB | PHE | A | 48 | 52.479 | 57.131 | 32.556 | 1.00 | 25.87 |
| 417 | CG | PHE | A | 48 | 53.188 | 57.147 | 33.878 | 1.00 | 25.55 |
| 418 | CD1 | PHE | A | 48 | 52.489 | 56.876 | 35.049 | 1.00 | 25.97 |
| 420 | CE1 | PHE | A | 48 | 53.131 | 56.864 | 36.274 | 1.00 | 25.51 |
| 422 | CZ | PHE | A | 48 | 54.480 | 57.116 | 36.349 | 1.00 | 25.34 |
| 424 | CE2 | PHE | A | 48 | 55.195 | 57.379 | 35.186 | 1.00 | 25.76 |
| 426 | CD2 | PHE | A | 48 | 54.551 | 57.383 | 33.959 | 1.00 | 24.78 |
| 428 | C | PHE | A | 48 | 51.323 | 55.730 | 30.787 | 1.00 | 25.98 |
| 429 | O | PHE | A | 48 | 50.987 | 56.762 | 30.226 | 1.00 | 25.18 |
| 430 | N | GLN | A | 49 | 51.222 | 54.528 | 30.221 | 1.00 | 26.46 |
| 432 | CA | GLN | A | 49 | 50.537 | 54.330 | 28.942 | 1.00 | 27.47 |
| 434 | CB | GLN | A | 49 | 50.502 | 52.854 | 28.527 | 1.00 | 27.56 |
| 437 | CG | GLN | A | 49 | 51.828 | 52.229 | 28.185 | 1.00 | 28.72 |
| 440 | CD | GLN | A | 49 | 52.596 | 52.968 | 27.106 | 1.00 | 30.09 |
| 441 | OE1 | GLN | A | 49 | 53.817 | 53.065 | 27.187 | 1.00 | 32.82 |
| 442 | NE2 | GLN | A | 49 | 51.897 | 53.475 | 26.096 | 1.00 | 30.99 |
| 445 | C | GLN | A | 49 | 49.111 | 54.786 | 29.106 | 1.00 | 28.28 |
| 446 | O | GLN | A | 49 | 48.511 | 54.598 | 30.172 | 1.00 | 28.52 |
| 447 | N | ASN | A | 50 | 48.579 | 55.403 | 28.060 | 1.00 | 28.97 |
| 449 | CA | ASN | A | 50 | 47.202 | 55.868 | 28.040 | 1.00 | 29.76 |
| 451 | CB | ASN | A | 50 | 46.212 | 54.687 | 28.180 | 1.00 | 30.31 |
| 454 | CG | ASN | A | 50 | 46.513 | 53.535 | 27.210 | 1.00 | 31.66 |
| 455 | OD1 | ASN | A | 50 | 46.576 | 53.726 | 25.997 | 1.00 | 36.40 |
| 456 | ND2 | ASN | A | 50 | 46.694 | 52.342 | 27.748 | 1.00 | 32.76 |
| 459 | C | ASN | A | 50 | 46.937 | 56.948 | 29.094 | 1.00 | 29.56 |
| 460 | O | ASN | A | 50 | 45.842 | 57.041 | 29.631 | 1.00 | 29.84 |
| 461 | N | THR | A | 51 | 47.958 | 57.750 | 29.393 | 1.00 | 29.02 |
| 463 | CA | THR | A | 51 | 47.782 | 59.023 | 30.090 | 1.00 | 28.55 |
| 465 | CB | THR | A | 51 | 48.663 | 59.090 | 31.346 | 1.00 | 28.99 |
| 467 | OG1 | THR | A | 51 | 50.045 | 59.094 | 30.966 | 1.00 | 29.70 |
| 469 | CG2 | THR | A | 51 | 48.504 | 57.836 | 32.213 | 1.00 | 29.52 |
| 473 | C | THR | A | 51 | 48.173 | 60.135 | 29.107 | 1.00 | 27.72 |
| 474 | O | THR | A | 51 | 48.886 | 59.861 | 28.147 | 1.00 | 27.59 |
| 475 | N | PRO | A | 52 | 47.713 | 61.371 | 29.316 | 1.00 | 26.46 |
| 476 | CA | PRO | A | 52 | 47.961 | 62.453 | 28.351 | 1.00 | 25.93 |
| 478 | CB | PRO | A | 52 | 47.404 | 63.699 | 29.061 | 1.00 | 25.92 |
| 481 | CG | PRO | A | 52 | 46.331 | 63.155 | 29.974 | 1.00 | 26.20 |
| 484 | CD | PRO | A | 52 | 46.879 | 61.831 | 30.447 | 1.00 | 26.74 |
| 487 | C | PRO | A | 52 | 49.419 | 62.688 | 27.918 | 1.00 | 25.28 |
| 488 | O | PRO | A | 52 | 49.638 | 62.912 | 26.731 | 1.00 | 24.82 |
| 489 | N | VAL | A | 53 | 50.389 | 62.661 | 28.824 | 1.00 | 24.84 |
| 491 | CA | VAL | A | 53 | 51.766 | 62.944 | 28.412 | 1.00 | 24.49 |
| 493 | CB | VAL | A | 53 | 52.711 | 63.189 | 29.616 | 1.00 | 24.35 |
| 495 | CG1 | VAL | A | 53 | 52.934 | 61.920 | 30.414 | 1.00 | 25.47 |
| 499 | CG2 | VAL | A | 53 | 54.047 | 63.752 | 29.131 | 1.00 | 25.13 |
| 503 | C | VAL | A | 53 | 52.317 | 61.860 | 27.460 | 1.00 | 23.84 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 504 | O | VAL | A | 53 | 52.962 | 62.172 | 26.462 | 1.00 | 23.42 |
| 505 | N | VAL | A | 54 | 52.046 | 60.594 | 27.752 | 1.00 | 23.38 |
| 507 | CA | VAL | A | 54 | 52.505 | 59.516 | 26.878 | 1.00 | 23.48 |
| 509 | CB | VAL | A | 54 | 52.449 | 58.146 | 27.567 | 1.00 | 23.07 |
| 511 | CG1 | VAL | A | 54 | 52.773 | 57.012 | 26.566 | 1.00 | 23.03 |
| 515 | CG2 | VAL | A | 54 | 53.409 | 58.125 | 28.740 | 1.00 | 23.55 |
| 519 | C | VAL | A | 54 | 51.725 | 59.512 | 25.567 | 1.00 | 23.67 |
| 520 | O | VAL | A | 54 | 52.297 | 59.299 | 24.510 | 1.00 | 23.73 |
| 521 | N | GLU | A | 55 | 50.427 | 59.782 | 25.632 | 1.00 | 23.99 |
| 523 | CA | GLU | A | 55 | 49.629 | 59.897 | 24.417 | 1.00 | 24.17 |
| 525 | CB | GLU | A | 55 | 48.155 | 60.087 | 24.761 | 1.00 | 24.86 |
| 528 | CG | GLU | A | 55 | 47.534 | 58.863 | 25.404 | 1.00 | 27.67 |
| 531 | CD | GLU | A | 55 | 46.125 | 59.115 | 25.899 | 1.00 | 33.01 |
| 532 | OE1 | GLU | A | 55 | 45.337 | 58.140 | 25.909 | 1.00 | 36.58 |
| 533 | OE2 | GLU | A | 55 | 45.806 | 60.274 | 26.278 | 1.00 | 35.89 |
| 534 | C | GLU | A | 55 | 50.115 | 61.066 | 23.562 | 1.00 | 22.99 |
| 535 | O | GLU | A | 55 | 50.099 | 60.980 | 22.345 | 1.00 | 21.91 |
| 536 | N | THR | A | 56 | 50.574 | 62.139 | 24.208 | 1.00 | 22.14 |
| 538 | CA | THR | A | 56 | 51.147 | 63.270 | 23.497 | 1.00 | 21.71 |
| 540 | CB | THR | A | 56 | 51.426 | 64.447 | 24.442 | 1.00 | 21.87 |
| 542 | OG1 | THR | A | 56 | 50.218 | 64.833 | 25.112 | 1.00 | 21.63 |
| 544 | CG2 | THR | A | 56 | 51.861 | 65.695 | 23.647 | 1.00 | 21.55 |
| 548 | C | THR | A | 56 | 52.435 | 62.833 | 22.813 | 1.00 | 21.19 |
| 549 | O | THR | A | 56 | 52.658 | 63.152 | 21.667 | 1.00 | 20.77 |
| 550 | N | MET | A | 57 | 53.268 | 62.075 | 23.515 | 1.00 | 21.45 |
| 552 | CA | MET | A | 57 | 54.525 | 61.583 | 22.936 | 1.00 | 21.16 |
| 554 | CB | MET | A | 57 | 55.321 | 60.768 | 23.965 | 1.00 | 21.28 |
| 557 | CG | MET | A | 57 | 55.825 | 61.558 | 25.165 | 1.00 | 21.06 |
| 560 | SD | MET | A | 57 | 56.503 | 60.485 | 26.448 | 1.00 | 21.92 |
| 561 | CE | MET | A | 57 | 58.036 | 59.941 | 25.581 | 1.00 | 18.94 |
| 565 | C | MET | A | 57 | 54.227 | 60.713 | 21.704 | 1.00 | 21.05 |
| 566 | O | MET | A | 57 | 54.873 | 60.858 | 20.676 | 1.00 | 21.01 |
| 567 | N | GLN | A | 58 | 53.228 | 59.835 | 21.812 | 1.00 | 21.04 |
| 569 | CA | GLN | A | 58 | 52.882 | 58.908 | 20.737 | 1.00 | 21.29 |
| 571 | CB | GLN | A | 58 | 51.862 | 57.889 | 21.229 | 1.00 | 21.77 |
| 574 | CG | GLN | A | 58 | 52.407 | 56.822 | 22.155 | 1.00 | 23.17 |
| 577 | CD | GLN | A | 58 | 51.297 | 55.954 | 22.728 | 1.00 | 26.61 |
| 578 | OE1 | GLN | A | 58 | 51.254 | 54.743 | 22.480 | 1.00 | 30.25 |
| 579 | NE2 | GLN | A | 58 | 50.389 | 56.569 | 23.474 | 1.00 | 24.83 |
| 582 | C | GLN | A | 58 | 52.299 | 59.642 | 19.526 | 1.00 | 21.06 |
| 583 | O | GLN | A | 58 | 52.547 | 59.291 | 18.371 | 1.00 | 19.85 |
| 584 | N | TYR | A | 59 | 51.495 | 60.656 | 19.804 | 1.00 | 20.82 |
| 586 | CA | TYR | A | 59 | 50.887 | 61.466 | 18.760 | 1.00 | 21.28 |
| 588 | CB | TYR | A | 59 | 49.946 | 62.447 | 19.433 | 1.00 | 21.43 |
| 591 | CG | TYR | A | 59 | 49.135 | 63.357 | 18.555 | 1.00 | 23.00 |
| 592 | CD1 | TYR | A | 59 | 47.838 | 63.002 | 18.154 | 1.00 | 24.56 |
| 594 | CE1 | TYR | A | 59 | 47.069 | 63.859 | 17.385 | 1.00 | 24.49 |
| 596 | CZ | TYR | A | 59 | 47.562 | 65.107 | 17.052 | 1.00 | 25.48 |
| 597 | OH | TYR | A | 59 | 46.793 | 65.965 | 16.292 | 1.00 | 24.53 |
| 599 | CE2 | TYR | A | 59 | 48.844 | 65.484 | 17.445 | 1.00 | 23.07 |
| 601 | CD2 | TYR | A | 59 | 49.604 | 64.618 | 18.212 | 1.00 | 23.55 |
| 603 | C | TYR | A | 59 | 51.967 | 62.218 | 18.002 | 1.00 | 20.79 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 604 | O | TYR | A | 59 | 52.033 | 62.184 | 16.765 | 1.00 | 20.35 |
| 605 | N | GLY | A | 60 | 52.811 | 62.910 | 18.761 | 1.00 | 20.69 |
| 607 | CA | GLY | A | 60 | 53.840 | 63.751 | 18.187 | 1.00 | 20.90 |
| 610 | C | GLY | A | 60 | 54.963 | 62.972 | 17.526 | 1.00 | 21.30 |
| 611 | O | GLY | A | 60 | 55.596 | 63.495 | 16.627 | 1.00 | 21.54 |
| 612 | N | ALA | A | 61 | 55.215 | 61.732 | 17.955 | 1.00 | 21.95 |
| 614 | CA | ALA | A | 61 | 56.315 | 60.942 | 17.389 | 1.00 | 22.16 |
| 616 | CB | ALA | A | 61 | 56.981 | 60.100 | 18.480 | 1.00 | 22.04 |
| 620 | C | ALA | A | 61 | 55.862 | 60.033 | 16.242 | 1.00 | 22.84 |
| 621 | O | ALA | A | 61 | 56.609 | 59.808 | 15.282 | 1.00 | 22.77 |
| 622 | N | LEU | A | 62 | 54.645 | 59.506 | 16.337 | 1.00 | 23.82 |
| 624 | CA | LEU | A | 62 | 54.227 | 58.413 | 15.446 | 1.00 | 25.01 |
| 626 | CB | LEU | A | 62 | 53.718 | 57.229 | 16.272 | 1.00 | 25.40 |
| 629 | CG | LEU | A | 62 | 54.803 | 56.448 | 16.999 | 1.00 | 26.02 |
| 631 | CD1 | LEU | A | 62 | 54.192 | 55.617 | 18.110 | 1.00 | 27.58 |
| 635 | CD2 | LEU | A | 62 | 55.583 | 55.570 | 16.011 | 1.00 | 26.63 |
| 639 | C | LEU | A | 62 | 53.188 | 58.758 | 14.386 | 1.00 | 25.71 |
| 640 | O | LEU | A | 62 | 53.144 | 58.088 | 13.352 | 1.00 | 25.79 |
| 641 | N | LEU | A | 63 | 52.351 | 59.772 | 14.626 | 1.00 | 26.23 |
| 643 | CA | LEU | A | 63 | 51.244 | 60.076 | 13.712 | 1.00 | 26.84 |
| 645 | CB | LEU | A | 63 | 50.045 | 60.627 | 14.487 | 1.00 | 27.25 |
| 648 | CG | LEU | A | 63 | 48.675 | 60.380 | 13.836 | 1.00 | 29.61 |
| 650 | CD1 | LEU | A | 63 | 48.417 | 58.886 | 13.617 | 1.00 | 30.97 |
| 654 | CD2 | LEU | A | 63 | 47.544 | 60.990 | 14.672 | 1.00 | 31.15 |
| 658 | C | LEU | A | 63 | 51.660 | 61.041 | 12.589 | 1.00 | 26.56 |
| 659 | O | LEU | A | 63 | 51.650 | 62.260 | 12.762 | 1.00 | 26.92 |
| 660 | N | GLY | A | 64 | 52.014 | 60.471 | 11.441 | 1.00 | 26.04 |
| 662 | CA | GLY | A | 64 | 52.480 | 61.230 | 10.294 | 1.00 | 25.24 |
| 665 | C | GLY | A | 64 | 53.983 | 61.421 | 10.347 | 1.00 | 24.44 |
| 666 | O | GLY | A | 64 | 54.635 | 61.015 | 11.301 | 1.00 | 24.64 |
| 667 | N | GLY | A | 65 | 54.513 | 62.081 | 9.331 | 1.00 | 23.73 |
| 669 | CA | GLY | A | 65 | 55.938 | 62.322 | 9.195 | 1.00 | 23.06 |
| 672 | C | GLY | A | 65 | 56.553 | 61.359 | 8.209 | 1.00 | 22.26 |
| 673 | O | GLY | A | 65 | 56.162 | 60.194 | 8.133 | 1.00 | 22.42 |
| 674 | N | LYS | A | 66 | 57.547 | 61.842 | 7.478 | 1.00 | 22.13 |
| 676 | CA | LYS | A | 66 | 58.154 | 61.112 | 6.374 | 1.00 | 21.99 |
| 678 | CB | LYS | A | 66 | 58.759 | 62.101 | 5.373 | 1.00 | 22.38 |
| 681 | CG | LYS | A | 66 | 57.740 | 63.053 | 4.741 | 1.00 | 22.42 |
| 684 | CD | LYS | A | 66 | 58.397 | 63.946 | 3.700 | 1.00 | 22.36 |
| 687 | CE | LYS | A | 66 | 59.309 | 65.000 | 4.315 | 1.00 | 22.65 |
| 690 | NZ | LYS | A | 66 | 58.610 | 65.764 | 5.390 | 1.00 | 22.32 |
| 694 | C | LYS | A | 66 | 59.236 | 60.121 | 6.820 | 1.00 | 21.22 |
| 695 | O | LYS | A | 66 | 59.639 | 59.250 | 6.044 | 1.00 | 21.45 |
| 696 | N | ARG | A | 67 | 59.679 | 60.268 | 8.064 | 1.00 | 20.48 |
| 698 | CA | ARG | A | 67 | 60.763 | 59.494 | 8.657 | 1.00 | 19.82 |
| 700 | CB | ARG | A | 67 | 60.347 | 58.035 | 8.877 | 1.00 | 19.66 |
| 703 | CG | ARG | A | 67 | 59.138 | 57.855 | 9.723 | 1.00 | 20.10 |
| 706 | CD | ARG | A | 67 | 59.272 | 58.230 | 11.192 | 1.00 | 20.40 |
| 709 | NE | ARG | A | 67 | 57.948 | 58.049 | 11.781 | 1.00 | 20.92 |
| 711 | CZ | ARG | A | 67 | 57.037 | 58.991 | 11.934 | 1.00 | 22.13 |
| 712 | NH1 | ARG | A | 67 | 57.298 | 60.255 | 11.645 | 1.00 | 23.06 |
| 715 | NH2 | ARG | A | 67 | 55.840 | 58.667 | 12.421 | 1.00 | 22.86 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 718 | C | ARG | A | 67 | 62.061 | 59.514 | 7.860 | 1.00 | 19.24 |
| 719 | O | ARG | A | 67 | 62.738 | 58.501 | 7.779 | 1.00 | 18.48 |
| 720 | N | LEU | A | 68 | 62.432 | 60.666 | 7.307 | 1.00 | 18.87 |
| 722 | CA | LEU | A | 68 | 63.630 | 60.734 | 6.485 | 1.00 | 18.40 |
| 724 | CB | LEU | A | 68 | 63.643 | 61.988 | 5.629 | 1.00 | 18.86 |
| 727 | CG | LEU | A | 68 | 62.430 | 62.083 | 4.708 | 1.00 | 18.30 |
| 729 | CD1 | LEU | A | 68 | 62.550 | 63.320 | 3.821 | 1.00 | 18.04 |
| 733 | CD2 | LEU | A | 68 | 62.266 | 60.815 | 3.896 | 1.00 | 19.13 |
| 737 | C | LEU | A | 68 | 64.908 | 60.646 | 7.296 | 1.00 | 18.46 |
| 738 | O | LEU | A | 68 | 65.933 | 60.241 | 6.772 | 1.00 | 18.88 |
| 739 | N | ARG | A | 69 | 64.866 | 61.017 | 8.562 | 1.00 | 17.65 |
| 741 | CA | ARG | A | 69 | 66.054 | 60.871 | 9.384 | 1.00 | 17.87 |
| 743 | CB | ARG | A | 69 | 66.000 | 61.756 | 10.611 | 1.00 | 17.85 |
| 746 | CG | ARG | A | 69 | 66.045 | 63.219 | 10.223 | 1.00 | 17.38 |
| 749 | CD | ARG | A | 69 | 65.459 | 64.177 | 11.253 | 1.00 | 17.84 |
| 752 | NE | ARG | A | 69 | 65.361 | 65.533 | 10.704 | 1.00 | 19.01 |
| 754 | CZ | ARG | A | 69 | 64.417 | 65.941 | 9.863 | 1.00 | 20.05 |
| 755 | NH1 | ARG | A | 69 | 64.422 | 67.193 | 9.411 | 1.00 | 22.90 |
| 758 | NH2 | ARG | A | 69 | 63.449 | 65.123 | 9.477 | 1.00 | 21.09 |
| 761 | C | ARG | A | 69 | 66.322 | 59.401 | 9.705 | 1.00 | 17.71 |
| 762 | O | ARG | A | 69 | 67.454 | 58.951 | 9.531 | 1.00 | 18.10 |
| 763 | N | PRO | A | 70 | 65.329 | 58.645 | 10.163 | 1.00 | 17.51 |
| 764 | CA | PRO | A | 70 | 65.476 | 57.180 | 10.192 | 1.00 | 17.45 |
| 766 | CB | PRO | A | 70 | 64.070 | 56.703 | 10.531 | 1.00 | 17.56 |
| 769 | CG | PRO | A | 70 | 63.506 | 57.791 | 11.356 | 1.00 | 17.73 |
| 772 | CD | PRO | A | 70 | 64.052 | 59.064 | 10.767 | 1.00 | 17.18 |
| 775 | C | PRO | A | 70 | 65.936 | 56.615 | 8.859 | 1.00 | 17.33 |
| 776 | O | PRO | A | 70 | 66.816 | 55.755 | 8.854 | 1.00 | 17.25 |
| 777 | N | PHE | A | 71 | 65.376 | 57.104 | 7.754 | 1.00 | 17.93 |
| 779 | CA | PHE | A | 71 | 65.781 | 56.677 | 6.427 | 1.00 | 18.40 |
| 781 | CB | PHE | A | 71 | 65.044 | 57.457 | 5.338 | 1.00 | 19.10 |
| 784 | CG | PHE | A | 71 | 65.198 | 56.872 | 3.941 | 1.00 | 19.82 |
| 785 | CD1 | PHE | A | 71 | 66.425 | 56.898 | 3.278 | 1.00 | 21.48 |
| 787 | CE1 | PHE | A | 71 | 66.558 | 56.356 | 1.990 | 1.00 | 24.16 |
| 789 | CZ | PHE | A | 71 | 65.456 | 55.801 | 1.354 | 1.00 | 23.70 |
| 791 | CE2 | PHE | A | 71 | 64.232 | 55.787 | 2.000 | 1.00 | 24.40 |
| 793 | CD2 | PHE | A | 71 | 64.112 | 56.329 | 3.289 | 1.00 | 21.85 |
| 795 | C | PHE | A | 71 | 67.288 | 56.831 | 6.274 | 1.00 | 18.39 |
| 796 | O | PHE | A | 71 | 67.951 | 55.920 | 5.814 | 1.00 | 18.40 |
| 797 | N | LEU | A | 72 | 67.820 | 57.973 | 6.683 | 1.00 | 18.52 |
| 799 | CA | LEU | A | 72 | 69.255 | 58.228 | 6.643 | 1.00 | 18.77 |
| 801 | CB | LEU | A | 72 | 69.554 | 59.650 | 7.101 | 1.00 | 19.16 |
| 804 | CG | LEU | A | 72 | 69.280 | 60.737 | 6.070 | 1.00 | 20.56 |
| 806 | CD1 | LEU | A | 72 | 69.409 | 62.108 | 6.739 | 1.00 | 21.70 |
| 810 | CD2 | LEU | A | 72 | 70.233 | 60.611 | 4.897 | 1.00 | 21.14 |
| 814 | C | LEU | A | 72 | 70.063 | 57.274 | 7.512 | 1.00 | 18.22 |
| 815 | O | LEU | A | 72 | 71.162 | 56.862 | 7.131 | 1.00 | 17.84 |
| 816 | N | VAL | A | 73 | 69.546 | 56.973 | 8.693 | 1.00 | 16.88 |
| 818 | CA | VAL | A | 73 | 70.235 | 56.066 | 9.609 | 1.00 | 17.06 |
| 820 | CB | VAL | A | 73 | 69.512 | 56.001 | 10.969 | 1.00 | 16.98 |
| 822 | CG1 | VAL | A | 73 | 70.075 | 54.909 | 11.865 | 1.00 | 17.14 |
| 826 | CG2 | VAL | A | 73 | 69.621 | 57.337 | 11.679 | 1.00 | 16.69 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 830 | C | VAL | A | 73 | 70.315 | 54.667 | 8.984 | 1.00 | 17.43 |
| 831 | O | VAL | A | 73 | 71.391 | 54.087 | 8.924 | 1.00 | 16.85 |
| 832 | N | TYR | A | 74 | 69.171 | 54.175 | 8.504 | 1.00 | 17.82 |
| 834 | CA | TYR | A | 74 | 69.049 | 52.853 | 7.890 | 1.00 | 18.73 |
| 836 | CB | TYR | A | 74 | 67.590 | 52.546 | 7.534 | 1.00 | 18.65 |
| 839 | CG | TYR | A | 74 | 66.682 | 52.294 | 8.706 | 1.00 | 17.77 |
| 840 | CD1 | TYR | A | 74 | 66.993 | 51.343 | 9.670 | 1.00 | 18.53 |
| 842 | CE1 | TYR | A | 74 | 66.152 | 51.109 | 10.734 | 1.00 | 19.24 |
| 844 | CZ | TYR | A | 74 | 64.967 | 51.819 | 10.844 | 1.00 | 17.86 |
| 845 | OH | TYR | A | 74 | 64.123 | 51.616 | 11.915 | 1.00 | 16.87 |
| 847 | CE2 | TYR | A | 74 | 64.650 | 52.774 | 9.914 | 1.00 | 18.34 |
| 849 | CD2 | TYR | A | 74 | 65.492 | 52.988 | 8.835 | 1.00 | 18.14 |
| 851 | C | TYR | A | 74 | 69.878 | 52.741 | 6.626 | 1.00 | 19.22 |
| 852 | O | TYR | A | 74 | 70.627 | 51.788 | 6.466 | 1.00 | 20.65 |
| 853 | N | ALA | A | 75 | 69.762 | 53.725 | 5.744 | 1.00 | 19.41 |
| 855 | CA | ALA | A | 75 | 70.470 | 53.707 | 4.474 | 1.00 | 19.53 |
| 857 | CB | ALA | A | 75 | 70.035 | 54.875 | 3.616 | 1.00 | 20.02 |
| 861 | C | ALA | A | 75 | 71.975 | 53.744 | 4.695 | 1.00 | 20.18 |
| 862 | O | ALA | A | 75 | 72.721 | 53.053 | 4.011 | 1.00 | 21.39 |
| 863 | N | THR | A | 76 | 72.423 | 54.545 | 5.656 | 1.00 | 20.00 |
| 865 | CA | THR | A | 76 | 73.841 | 54.656 | 5.930 | 1.00 | 20.26 |
| 867 | CB | THR | A | 76 | 74.124 | 55.842 | 6.828 | 1.00 | 20.06 |
| 869 | OG1 | THR | A | 76 | 73.742 | 57.060 | 6.143 | 1.00 | 19.95 |
| 871 | CG2 | THR | A | 76 | 75.624 | 55.979 | 7.077 | 1.00 | 20.73 |
| 875 | C | THR | A | 76 | 74.371 | 53.370 | 6.527 | 1.00 | 20.27 |
| 876 | O | THR | A | 76 | 75.330 | 52.821 | 6.025 | 1.00 | 20.97 |
| 877 | N | GLY | A | 77 | 73.743 | 52.886 | 7.588 | 1.00 | 20.36 |
| 879 | CA | GLY | A | 77 | 74.136 | 51.630 | 8.199 | 1.00 | 20.44 |
| 882 | C | GLY | A | 77 | 74.090 | 50.470 | 7.229 | 1.00 | 20.43 |
| 883 | O | GLY | A | 77 | 74.966 | 49.600 | 7.242 | 1.00 | 21.38 |
| 884 | N | HIS | A | 78 | 73.061 | 50.442 | 6.393 | 1.00 | 21.26 |
| 886 | CA | HIS | A | 78 | 72.886 | 49.367 | 5.401 | 1.00 | 21.95 |
| 888 | CB | HIS | A | 78 | 71.577 | 49.530 | 4.623 | 1.00 | 22.16 |
| 891 | CG | HIS | A | 78 | 70.369 | 49.049 | 5.362 | 1.00 | 21.95 |
| 892 | ND1 | HIS | A | 78 | 69.094 | 49.468 | 5.051 | 1.00 | 23.29 |
| 894 | CE1 | HIS | A | 78 | 68.231 | 48.892 | 5.869 | 1.00 | 23.63 |
| 896 | NE2 | HIS | A | 78 | 68.899 | 48.097 | 6.687 | 1.00 | 21.16 |
| 898 | CD2 | HIS | A | 78 | 70.238 | 48.181 | 6.394 | 1.00 | 22.72 |
| 900 | C | HIS | A | 78 | 74.054 | 49.313 | 4.421 | 1.00 | 22.56 |
| 901 | O | HIS | A | 78 | 74.455 | 48.228 | 3.995 | 1.00 | 21.64 |
| 902 | N | MET | A | 79 | 74.610 | 50.477 | 4.080 | 1.00 | 23.05 |
| 904 | CA | MET | A | 79 | 75.782 | 50.536 | 3.201 | 1.00 | 23.89 |
| 906 | CB | MET | A | 79 | 76.282 | 51.961 | 3.027 | 1.00 | 24.12 |
| 909 | CG | MET | A | 79 | 75.546 | 52.765 | 2.016 | 1.00 | 26.38 |
| 912 | SD | MET | A | 79 | 76.590 | 54.090 | 1.347 | 1.00 | 31.06 |
| 913 | CE | MET | A | 79 | 77.179 | 54.849 | 2.837 | 1.00 | 30.61 |
| 917 | C | MET | A | 79 | 76.944 | 49.713 | 3.732 | 1.00 | 24.04 |
| 918 | O | MET | A | 79 | 77.740 | 49.208 | 2.945 | 1.00 | 24.70 |
| 919 | N | PHE | A | 80 | 77.052 | 49.617 | 5.057 | 1.00 | 24.12 |
| 921 | CA | PHE | A | 80 | 78.122 | 48.863 | 5.723 | 1.00 | 24.15 |
| 923 | CB | PHE | A | 80 | 78.644 | 49.693 | 6.881 | 1.00 | 24.28 |
| 926 | CG | PHE | A | 80 | 79.127 | 51.040 | 6.455 | 1.00 | 25.09 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 927 | CD1 | PHE | A | 80 | 78.410 | 52.183 | 6.759 | 1.00 | 25.88 |
| 929 | CE1 | PHE | A | 80 | 78.847 | 53.424 | 6.357 | 1.00 | 25.67 |
| 931 | CZ | PHE | A | 80 | 80.015 | 53.547 | 5.641 | 1.00 | 26.11 |
| 933 | CE2 | PHE | A | 80 | 80.751 | 52.415 | 5.330 | 1.00 | 26.51 |
| 935 | CD2 | PHE | A | 80 | 80.305 | 51.167 | 5.736 | 1.00 | 26.10 |
| 937 | C | PHE | A | 80 | 77.710 | 47.461 | 6.196 | 1.00 | 24.09 |
| 938 | O | PHE | A | 80 | 78.475 | 46.770 | 6.875 | 1.00 | 23.88 |
| 939 | N | GLY | A | 81 | 76.508 | 47.039 | 5.815 | 1.00 | 23.45 |
| 941 | CA | GLY | A | 81 | 76.025 | 45.708 | 6.114 | 1.00 | 23.38 |
| 944 | C | GLY | A | 81 | 75.544 | 45.539 | 7.545 | 1.00 | 23.11 |
| 945 | O | GLY | A | 81 | 75.412 | 44.415 | 8.032 | 1.00 | 22.14 |
| 946 | N | VAL | A | 82 | 75.261 | 46.636 | 8.241 | 1.00 | 22.50 |
| 948 | CA | VAL | A | 82 | 74.698 | 46.461 | 9.577 | 1.00 | 22.69 |
| 950 | CB | VAL | A | 82 | 75.093 | 47.576 | 10.642 | 1.00 | 22.92 |
| 952 | CG1 | VAL | A | 82 | 75.915 | 48.711 | 10.067 | 1.00 | 23.76 |
| 956 | CG2 | VAL | A | 82 | 73.908 | 48.074 | 11.396 | 1.00 | 22.71 |
| 960 | C | VAL | A | 82 | 73.194 | 46.144 | 9.484 | 1.00 | 21.96 |
| 961 | O | VAL | A | 82 | 72.487 | 46.604 | 8.591 | 1.00 | 21.42 |
| 962 | N | SER | A | 83 | 72.746 | 45.302 | 10.402 | 1.00 | 21.48 |
| 964 | CA | SER | A | 83 | 71.389 | 44.778 | 10.405 | 1.00 | 21.77 |
| 966 | CB | SER | A | 83 | 71.250 | 43.671 | 11.467 | 1.00 | 22.01 |
| 969 | OG | SER | A | 83 | 69.901 | 43.269 | 11.656 | 1.00 | 24.55 |
| 971 | C | SER | A | 83 | 70.388 | 45.893 | 10.669 | 1.00 | 21.66 |
| 972 | O | SER | A | 83 | 70.614 | 46.768 | 11.497 | 1.00 | 20.52 |
| 973 | N | THR | A | 84 | 69.280 | 45.849 | 9.950 | 1.00 | 21.30 |
| 975 | CA | THR | A | 84 | 68.197 | 46.782 | 10.145 | 1.00 | 21.37 |
| 977 | CB | THR | A | 84 | 67.041 | 46.395 | 9.243 | 1.00 | 21.59 |
| 979 | OG1 | THR | A | 84 | 67.522 | 46.238 | 7.898 | 1.00 | 20.65 |
| 981 | CG2 | THR | A | 84 | 66.004 | 47.531 | 9.175 | 1.00 | 21.88 |
| 985 | C | THR | A | 84 | 67.742 | 46.839 | 11.609 | 1.00 | 21.40 |
| 986 | O | THR | A | 84 | 67.457 | 47.919 | 12.127 | 1.00 | 20.26 |
| 987 | N | ASN | A | 85 | 67.712 | 45.681 | 12.273 | 1.00 | 20.85 |
| 989 | CA | ASN | A | 85 | 67.259 | 45.592 | 13.665 | 1.00 | 21.11 |
| 991 | CB | ASN | A | 85 | 67.155 | 44.113 | 14.110 | 1.00 | 20.78 |
| 994 | CG | ASN | A | 85 | 66.777 | 43.962 | 15.577 | 1.00 | 20.57 |
| 995 | OD1 | ASN | A | 85 | 65.629 | 44.176 | 15.960 | 1.00 | 20.74 |
| 996 | ND2 | ASN | A | 85 | 67.741 | 43.572 | 16.395 | 1.00 | 21.96 |
| 999 | C | ASN | A | 85 | 68.135 | 46.366 | 14.648 | 1.00 | 21.18 |
| 1000 | O | ASN | A | 85 | 67.630 | 46.935 | 15.589 | 1.00 | 21.24 |
| 1001 | N | THR | A | 86 | 69.445 | 46.363 | 14.445 | 1.00 | 21.31 |
| 1003 | CA | THR | A | 86 | 70.325 | 47.176 | 15.288 | 1.00 | 22.18 |
| 1005 | CB | THR | A | 86 | 71.831 | 46.719 | 15.233 | 1.00 | 23.07 |
| 1007 | OG1 | THR | A | 86 | 72.729 | 47.845 | 15.254 | 1.00 | 25.14 |
| 1009 | CG2 | THR | A | 86 | 72.163 | 46.051 | 13.972 | 1.00 | 25.36 |
| 1013 | C | THR | A | 86 | 70.149 | 48.653 | 14.952 | 1.00 | 21.28 |
| 1014 | O | THR | A | 86 | 70.191 | 49.488 | 15.836 | 1.00 | 21.18 |
| 1015 | N | LEU | A | 87 | 69.889 | 48.958 | 13.685 | 1.00 | 20.13 |
| 1017 | CA | LEU | A | 87 | 69.699 | 50.338 | 13.267 | 1.00 | 19.67 |
| 1019 | CB | LEU | A | 87 | 69.773 | 50.458 | 11.743 | 1.00 | 19.03 |
| 1022 | CG | LEU | A | 87 | 71.174 | 50.220 | 11.203 | 1.00 | 20.05 |
| 1024 | CD1 | LEU | A | 87 | 71.133 | 49.777 | 9.747 | 1.00 | 20.55 |
| 1028 | CD2 | LEU | A | 87 | 72.025 | 51.477 | 11.362 | 1.00 | 21.66 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 1032 | C | LEU | A | 87 | 68.395 | 50.943 | 13.785 | 1.00 | 19.10 |
| 1033 | O | LEU | A | 87 | 68.266 | 52.154 | 13.797 | 1.00 | 17.73 |
| 1034 | N | ASP | A | 88 | 67.452 | 50.098 | 14.213 | 1.00 | 18.92 |
| 1036 | CA | ASP | A | 88 | 66.206 | 50.555 | 14.808 | 1.00 | 19.26 |
| 1038 | CB | ASP | A | 88 | 65.374 | 49.380 | 15.347 | 1.00 | 19.80 |
| 1041 | CG | ASP | A | 88 | 64.537 | 48.689 | 14.279 | 1.00 | 21.07 |
| 1042 | OD1 | ASP | A | 88 | 64.370 | 49.232 | 13.167 | 1.00 | 22.88 |
| 1043 | OD2 | ASP | A | 88 | 63.977 | 47.584 | 14.496 | 1.00 | 22.05 |
| 1044 | C | ASP | A | 88 | 66.491 | 51.503 | 15.972 | 1.00 | 18.72 |
| 1045 | O | ASP | A | 88 | 65.743 | 52.455 | 16.193 | 1.00 | 18.90 |
| 1046 | N | ALA | A | 89 | 67.551 | 51.227 | 16.724 | 1.00 | 18.47 |
| 1048 | CA | ALA | A | 89 | 67.879 | 52.031 | 17.902 | 1.00 | 18.05 |
| 1050 | CB | ALA | A | 89 | 68.957 | 51.350 | 18.777 | 1.00 | 18.08 |
| 1054 | C | ALA | A | 89 | 68.262 | 53.464 | 17.528 | 1.00 | 17.75 |
| 1055 | O | ALA | A | 89 | 67.571 | 54.391 | 17.954 | 1.00 | 16.58 |
| 1056 | N | PRO | A | 90 | 69.334 | 53.674 | 16.754 | 1.00 | 17.46 |
| 1057 | CA | PRO | A | 90 | 69.660 | 55.034 | 16.310 | 1.00 | 17.24 |
| 1059 | CB | PRO | A | 90 | 70.978 | 54.870 | 15.537 | 1.00 | 17.48 |
| 1062 | CG | PRO | A | 90 | 71.073 | 53.397 | 15.176 | 1.00 | 17.90 |
| 1065 | CD | PRO | A | 90 | 70.318 | 52.690 | 16.274 | 1.00 | 17.39 |
| 1068 | C | PRO | A | 90 | 68.570 | 55.674 | 15.452 | 1.00 | 17.54 |
| 1069 | O | PRO | A | 90 | 68.372 | 56.871 | 15.546 | 1.00 | 16.99 |
| 1070 | N | ALA | A | 91 | 67.881 | 54.899 | 14.617 | 1.00 | 17.55 |
| 1072 | CA | ALA | A | 91 | 66.786 | 55.439 | 13.827 | 1.00 | 17.51 |
| 1074 | CB | ALA | A | 91 | 66.196 | 54.371 | 12.908 | 1.00 | 17.15 |
| 1078 | C | ALA | A | 91 | 65.710 | 56.010 | 14.751 | 1.00 | 17.33 |
| 1079 | O | ALA | A | 91 | 65.235 | 57.120 | 14.540 | 1.00 | 17.48 |
| 1080 | N | ALA | A | 92 | 65.365 | 55.276 | 15.797 | 1.00 | 17.28 |
| 1082 | CA | ALA | A | 92 | 64.309 | 55.702 | 16.702 | 1.00 | 17.98 |
| 1084 | CB | ALA | A | 92 | 63.858 | 54.558 | 17.575 | 1.00 | 17.95 |
| 1088 | C | ALA | A | 92 | 64.764 | 56.881 | 17.559 | 1.00 | 18.07 |
| 1089 | O | ALA | A | 92 | 63.986 | 57.800 | 17.828 | 1.00 | 18.55 |
| 1090 | N | ALA | A | 93 | 66.027 | 56.852 | 17.965 | 1.00 | 17.63 |
| 1092 | CA | ALA | A | 93 | 66.612 | 57.905 | 18.776 | 1.00 | 17.90 |
| 1094 | CB | ALA | A | 93 | 68.016 | 57.551 | 19.129 | 1.00 | 17.89 |
| 1098 | C | ALA | A | 93 | 66.602 | 59.238 | 18.046 | 1.00 | 18.01 |
| 1099 | O | ALA | A | 93 | 66.199 | 60.258 | 18.611 | 1.00 | 16.96 |
| 1100 | N | VAL | A | 94 | 67.076 | 59.233 | 16.802 | 1.00 | 18.36 |
| 1102 | CA | VAL | A | 94 | 67.108 | 60.469 | 16.022 | 1.00 | 19.02 |
| 1104 | CB | VAL | A | 94 | 67.919 | 60.359 | 14.706 | 1.00 | 19.48 |
| 1106 | CG1 | VAL | A | 94 | 69.346 | 59.943 | 15.004 | 1.00 | 21.38 |
| 1110 | CG2 | VAL | A | 94 | 67.262 | 59.431 | 13.694 | 1.00 | 20.88 |
| 1114 | C | VAL | A | 94 | 65.697 | 60.984 | 15.728 | 1.00 | 18.91 |
| 1115 | O | VAL | A | 94 | 65.478 | 62.192 | 15.694 | 1.00 | 19.41 |
| 1116 | N | GLU | A | 95 | 64.755 | 60.075 | 15.506 | 1.00 | 18.77 |
| 1118 | CA | GLU | A | 95 | 63.371 | 60.460 | 15.281 | 1.00 | 19.03 |
| 1120 | CB | GLU | A | 95 | 62.580 | 59.307 | 14.672 | 1.00 | 19.35 |
| 1123 | CG | GLU | A | 95 | 61.202 | 59.659 | 14.140 | 1.00 | 20.47 |
| 1126 | CD | GLU | A | 95 | 61.187 | 60.686 | 13.014 | 1.00 | 23.08 |
| 1127 | OE1 | GLU | A | 95 | 60.085 | 61.188 | 12.699 | 1.00 | 21.79 |
| 1128 | OE2 | GLU | A | 95 | 62.243 | 61.001 | 12.436 | 1.00 | 22.95 |
| 1129 | C | GLU | A | 95 | 62.726 | 60.972 | 16.571 | 1.00 | 19.06 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 1130 | O | GLU | A | 95 | 61.883 | 61.856 | 16.515 | 1.00 | 18.98 |
| 1131 | N | CYS | A | 96 | 63.154 | 60.466 | 17.724 | 1.00 | 19.07 |
| 1133 | CA | CYS | A | 96 | 62.684 | 61.026 | 18.999 | 1.00 | 19.48 |
| 1135 | CB | CYS | A | 96 | 63.154 | 60.218 | 20.204 | 1.00 | 19.62 |
| 1138 | SG | CYS | A | 96 | 62.240 | 58.692 | 20.462 | 1.00 | 21.40 |
| 1139 | C | CYS | A | 96 | 63.139 | 62.464 | 19.144 | 1.00 | 18.83 |
| 1140 | O | CYS | A | 96 | 62.348 | 63.311 | 19.526 | 1.00 | 19.11 |
| 1141 | N | ILE | A | 97 | 64.405 | 62.740 | 18.846 | 1.00 | 18.13 |
| 1143 | CA | ILE | A | 97 | 64.900 | 64.108 | 18.934 | 1.00 | 17.94 |
| 1145 | CB | ILE | A | 97 | 66.402 | 64.201 | 18.602 | 1.00 | 18.00 |
| 1147 | CG1 | ILE | A | 97 | 67.269 | 63.442 | 19.628 | 1.00 | 18.23 |
| 1150 | CD1 | ILE | A | 97 | 67.160 | 63.942 | 21.057 | 1.00 | 18.91 |
| 1154 | CG2 | ILE | A | 97 | 66.824 | 65.659 | 18.520 | 1.00 | 18.94 |
| 1158 | C | ILE | A | 97 | 64.117 | 64.994 | 17.959 | 1.00 | 17.15 |
| 1159 | O | ILE | A | 97 | 63.700 | 66.094 | 18.308 | 1.00 | 16.79 |
| 1160 | N | HIS | A | 98 | 63.952 | 64.506 | 16.732 | 1.00 | 16.32 |
| 1162 | CA | HIS | A | 98 | 63.238 | 65.238 | 15.701 | 1.00 | 16.58 |
| 1164 | CB | HIS | A | 98 | 63.182 | 64.438 | 14.409 | 1.00 | 16.65 |
| 1167 | CG | HIS | A | 98 | 62.424 | 65.119 | 13.321 | 1.00 | 16.27 |
| 1168 | ND1 | HIS | A | 98 | 61.352 | 64.536 | 12.675 | 1.00 | 17.53 |
| 1170 | CE1 | HIS | A | 98 | 60.892 | 65.378 | 11.761 | 1.00 | 15.88 |
| 1172 | NE2 | HIS | A | 98 | 61.620 | 66.480 | 11.800 | 1.00 | 17.29 |
| 1174 | CD2 | HIS | A | 98 | 62.573 | 66.348 | 12.779 | 1.00 | 15.01 |
| 1176 | C | HIS | A | 98 | 61.825 | 65.555 | 16.167 | 1.00 | 16.53 |
| 1177 | O | HIS | A | 98 | 61.399 | 66.712 | 16.151 | 1.00 | 16.57 |
| 1178 | N | ALA | A | 99 | 61.119 | 64.532 | 16.620 | 1.00 | 15.86 |
| 1180 | CA | ALA | A | 99 | 59.753 | 64.699 | 17.119 | 1.00 | 16.23 |
| 1182 | CB | ALA | A | 99 | 59.177 | 63.346 | 17.566 | 1.00 | 16.25 |
| 1186 | C | ALA | A | 99 | 59.671 | 65.720 | 18.251 | 1.00 | 16.36 |
| 1187 | O | ALA | A | 99 | 58.753 | 66.544 | 18.297 | 1.00 | 16.22 |
| 1188 | N | TYR | A | 100 | 60.632 | 65.668 | 19.168 | 1.00 | 16.81 |
| 1190 | CA | TYR | A | 100 | 60.653 | 66.585 | 20.289 | 1.00 | 17.25 |
| 1192 | CB | TYR | A | 100 | 61.742 | 66.187 | 21.312 | 1.00 | 18.09 |
| 1195 | CG | TYR | A | 100 | 62.785 | 67.233 | 21.639 | 1.00 | 18.65 |
| 1196 | CD1 | TYR | A | 100 | 62.444 | 68.391 | 22.309 | 1.00 | 20.51 |
| 1198 | CE1 | TYR | A | 100 | 63.388 | 69.341 | 22.613 | 1.00 | 22.48 |
| 1200 | CZ | TYR | A | 100 | 64.701 | 69.138 | 22.248 | 1.00 | 22.20 |
| 1201 | OH | TYR | A | 100 | 65.628 | 70.083 | 22.565 | 1.00 | 24.51 |
| 1203 | CE2 | TYR | A | 100 | 65.075 | 67.983 | 21.590 | 1.00 | 21.60 |
| 1205 | CD2 | TYR | A | 100 | 64.122 | 67.037 | 21.306 | 1.00 | 19.95 |
| 1207 | C | TYR | A | 100 | 60.837 | 68.001 | 19.766 | 1.00 | 17.28 |
| 1208 | O | TYR | A | 100 | 60.178 | 68.921 | 20.232 | 1.00 | 16.91 |
| 1209 | N | SER | A | 101 | 61.709 | 68.169 | 18.780 | 1.00 | 17.12 |
| 1211 | CA | SER | A | 101 | 62.028 | 69.486 | 18.281 | 1.00 | 17.61 |
| 1213 | CB | SER | A | 101 | 63.209 | 69.446 | 17.312 | 1.00 | 17.91 |
| 1216 | OG | SER | A | 101 | 62.859 | 68.946 | 16.045 | 1.00 | 19.03 |
| 1218 | C | SER | A | 101 | 60.787 | 70.161 | 17.665 | 1.00 | 18.18 |
| 1219 | O | SER | A | 101 | 60.591 | 71.367 | 17.826 | 1.00 | 17.08 |
| 1220 | N | LEU | A | 102 | 59.936 | 69.376 | 17.021 | 1.00 | 18.08 |
| 1222 | CA | LEU | A | 102 | 58.748 | 69.937 | 16.356 | 1.00 | 18.75 |
| 1224 | CB | LEU | A | 102 | 58.168 | 68.946 | 15.359 | 1.00 | 18.81 |
| 1227 | CG | LEU | A | 102 | 59.159 | 68.371 | 14.350 | 1.00 | 19.61 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 1229 | CD1 | LEU | A | 102 | 58.421 | 67.472 | 13.385 | 1.00 | 19.87 |
| 1233 | CD2 | LEU | A | 102 | 59.901 | 69.477 | 13.628 | 1.00 | 20.82 |
| 1237 | C | LEU | A | 102 | 57.676 | 70.285 | 17.371 | 1.00 | 18.79 |
| 1238 | O | LEU | A | 102 | 56.928 | 71.252 | 17.192 | 1.00 | 19.67 |
| 1239 | N | ILE | A | 103 | 57.581 | 69.478 | 18.422 | 1.00 | 18.80 |
| 1241 | CA | ILE | A | 103 | 56.574 | 69.704 | 19.448 | 1.00 | 18.69 |
| 1243 | CB | ILE | A | 103 | 56.590 | 68.612 | 20.520 | 1.00 | 18.23 |
| 1245 | CG1 | ILE | A | 103 | 56.062 | 67.307 | 19.941 | 1.00 | 17.66 |
| 1248 | CD1 | ILE | A | 103 | 56.017 | 66.149 | 20.924 | 1.00 | 19.38 |
| 1252 | CG2 | ILE | A | 103 | 55.756 | 69.050 | 21.746 | 1.00 | 18.51 |
| 1256 | C | ILE | A | 103 | 56.844 | 71.069 | 20.071 | 1.00 | 19.44 |
| 1257 | O | ILE | A | 103 | 55.925 | 71.851 | 20.233 | 1.00 | 19.55 |
| 1258 | N | HIS | A | 104 | 58.108 | 71.358 | 20.383 | 1.00 | 19.42 |
| 1260 | CA | HIS | A | 104 | 58.452 | 72.609 | 21.039 | 1.00 | 20.66 |
| 1262 | CB | HIS | A | 104 | 59.797 | 72.507 | 21.730 | 1.00 | 21.50 |
| 1265 | CG | HIS | A | 104 | 59.735 | 71.795 | 23.045 | 1.00 | 25.90 |
| 1266 | ND1 | HIS | A | 104 | 59.610 | 70.432 | 23.149 | 1.00 | 34.19 |
| 1268 | CE1 | HIS | A | 104 | 59.570 | 70.087 | 24.425 | 1.00 | 32.41 |
| 1270 | NE2 | HIS | A | 104 | 59.660 | 71.175 | 25.149 | 1.00 | 32.34 |
| 1272 | CD2 | HIS | A | 104 | 59.748 | 72.261 | 24.312 | 1.00 | 32.88 |
| 1274 | C | HIS | A | 104 | 58.437 | 73.774 | 20.072 | 1.00 | 20.22 |
| 1275 | O | HIS | A | 104 | 58.095 | 74.880 | 20.444 | 1.00 | 20.04 |
| 1276 | N | ASP | A | 105 | 58.809 | 73.500 | 18.829 | 1.00 | 20.34 |
| 1278 | CA | ASP | A | 105 | 58.834 | 74.488 | 17.772 | 1.00 | 20.27 |
| 1280 | CB | ASP | A | 105 | 59.394 | 73.845 | 16.496 | 1.00 | 20.14 |
| 1283 | CG | ASP | A | 105 | 59.438 | 74.806 | 15.326 | 1.00 | 19.89 |
| 1284 | OD1 | ASP | A | 105 | 58.542 | 74.720 | 14.458 | 1.00 | 20.18 |
| 1285 | OD2 | ASP | A | 105 | 60.332 | 75.665 | 15.194 | 1.00 | 18.02 |
| 1286 | C | ASP | A | 105 | 57.447 | 75.081 | 17.512 | 1.00 | 20.91 |
| 1287 | O | ASP | A | 105 | 57.322 | 76.277 | 17.253 | 1.00 | 21.26 |
| 1288 | N | ASP | A | 106 | 56.410 | 74.254 | 17.580 | 1.00 | 21.41 |
| 1290 | CA | ASP | A | 106 | 55.037 | 74.718 | 17.328 | 1.00 | 21.41 |
| 1292 | CB | ASP | A | 106 | 54.098 | 73.551 | 17.048 | 1.00 | 21.45 |
| 1295 | CG | ASP | A | 106 | 54.436 | 72.819 | 15.799 | 1.00 | 20.29 |
| 1296 | OD1 | ASP | A | 106 | 54.167 | 71.594 | 15.734 | 1.00 | 20.18 |
| 1297 | OD2 | ASP | A | 106 | 54.978 | 73.379 | 14.841 | 1.00 | 19.29 |
| 1298 | C | ASP | A | 106 | 54.428 | 75.500 | 18.483 | 1.00 | 21.71 |
| 1299 | O | ASP | A | 106 | 53.395 | 76.123 | 18.301 | 1.00 | 22.06 |
| 1300 | N | LEU | A | 107 | 55.039 | 75.467 | 19.664 | 1.00 | 21.73 |
| 1302 | CA | LEU | A | 107 | 54.463 | 76.129 | 20.837 | 1.00 | 21.71 |
| 1304 | CB | LEU | A | 107 | 55.389 | 76.027 | 22.052 | 1.00 | 21.29 |
| 1307 | CG | LEU | A | 107 | 55.643 | 74.639 | 22.631 | 1.00 | 21.02 |
| 1309 | CD1 | LEU | A | 107 | 56.681 | 74.748 | 23.744 | 1.00 | 21.63 |
| 1313 | CD2 | LEU | A | 107 | 54.375 | 73.987 | 23.130 | 1.00 | 21.37 |
| 1317 | C | LEU | A | 107 | 54.173 | 77.611 | 20.587 | 1.00 | 22.13 |
| 1318 | O | LEU | A | 107 | 54.852 | 78.255 | 19.795 | 1.00 | 21.48 |
| 1319 | N | PRO | A | 108 | 53.167 | 78.152 | 21.273 | 1.00 | 23.19 |
| 1320 | CA | PRO | A | 108 | 52.850 | 79.588 | 21.175 | 1.00 | 23.59 |
| 1322 | CB | PRO | A | 108 | 51.811 | 79.779 | 22.282 | 1.00 | 24.00 |
| 1325 | CG | PRO | A | 108 | 51.099 | 78.464 | 22.308 | 1.00 | 23.90 |
| 1328 | CD | PRO | A | 108 | 52.216 | 77.443 | 22.149 | 1.00 | 22.62 |
| 1331 | C | PRO | A | 108 | 54.045 | 80.533 | 21.348 | 1.00 | 24.21 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 1332 | O | PRO | A | 108 | 54.148 | 81.494 | 20.599 | 1.00 | 25.11 |
| 1333 | N | ALA | A | 109 | 54.943 | 80.255 | 22.285 | 1.00 | 24.74 |
| 1335 | CA | ALA | A | 109 | 56.123 | 81.094 | 22.516 | 1.00 | 25.23 |
| 1337 | CB | ALA | A | 109 | 56.753 | 80.737 | 23.867 | 1.00 | 25.78 |
| 1341 | C | ALA | A | 109 | 57.176 | 80.941 | 21.417 | 1.00 | 25.46 |
| 1342 | O | ALA | A | 109 | 58.093 | 81.742 | 21.317 | 1.00 | 24.70 |
| 1343 | N | MET | A | 110 | 57.053 | 79.879 | 20.626 | 1.00 | 25.19 |
| 1345 | CA | MET | A | 110 | 57.981 | 79.590 | 19.550 | 1.00 | 26.00 |
| 1347 | CB | MET | A | 110 | 58.362 | 78.109 | 19.598 | 1.00 | 25.79 |
| 1350 | CG | MET | A | 110 | 58.997 | 77.719 | 20.916 | 1.00 | 27.52 |
| 1353 | SD | MET | A | 110 | 60.690 | 78.194 | 20.987 | 1.00 | 31.55 |
| 1354 | CE | MET | A | 110 | 61.411 | 77.093 | 19.688 | 1.00 | 31.97 |
| 1358 | C | MET | A | 110 | 57.345 | 79.995 | 18.207 | 1.00 | 25.73 |
| 1359 | O | MET | A | 110 | 57.213 | 81.186 | 17.942 | 1.00 | 25.54 |
| 1360 | N | ASP | A | 111 | 56.937 | 79.038 | 17.374 | 1.00 | 25.29 |
| 1362 | CA | ASP | A | 111 | 56.373 | 79.388 | 16.061 | 1.00 | 25.81 |
| 1364 | CB | ASP | A | 111 | 56.832 | 78.419 | 14.969 | 1.00 | 25.24 |
| 1367 | CG | ASP | A | 111 | 58.319 | 78.496 | 14.716 | 1.00 | 24.83 |
| 1368 | OD1 | ASP | A | 111 | 58.853 | 77.642 | 13.954 | 1.00 | 22.09 |
| 1369 | OD2 | ASP | A | 111 | 59.049 | 79.364 | 15.253 | 1.00 | 25.62 |
| 1370 | C | ASP | A | 111 | 54.851 | 79.525 | 16.069 | 1.00 | 25.92 |
| 1371 | O | ASP | A | 111 | 54.289 | 80.054 | 15.126 | 1.00 | 26.07 |
| 1372 | N | ASP | A | 112 | 54.206 | 79.043 | 17.125 | 1.00 | 26.89 |
| 1374 | CA | ASP | A | 112 | 52.759 | 79.211 | 17.350 | 1.00 | 27.69 |
| 1376 | CB | ASP | A | 112 | 52.419 | 80.670 | 17.671 | 1.00 | 28.12 |
| 1379 | CG | ASP | A | 112 | 51.000 | 80.840 | 18.202 | 1.00 | 29.63 |
| 1380 | OD1 | ASP | A | 112 | 50.458 | 81.960 | 18.094 | 1.00 | 31.75 |
| 1381 | OD2 | ASP | A | 112 | 50.342 | 79.911 | 18.732 | 1.00 | 31.76 |
| 1382 | C | ASP | A | 112 | 51.952 | 78.715 | 16.157 | 1.00 | 28.05 |
| 1383 | O | ASP | A | 112 | 51.159 | 79.450 | 15.549 | 1.00 | 28.01 |
| 1384 | N | ASP | A | 113 | 52.190 | 77.456 | 15.809 | 1.00 | 28.07 |
| 1386 | CA | ASP | A | 113 | 51.534 | 76.822 | 14.686 | 1.00 | 27.99 |
| 1388 | CB | ASP | A | 113 | 52.553 | 76.037 | 13.855 | 1.00 | 28.56 |
| 1391 | CG | ASP | A | 113 | 53.069 | 76.830 | 12.677 | 1.00 | 29.78 |
| 1392 | OD1 | ASP | A | 113 | 52.257 | 77.111 | 11.774 | 1.00 | 33.36 |
| 1393 | OD2 | ASP | A | 113 | 54.255 | 77.210 | 12.549 | 1.00 | 31.90 |
| 1394 | C | ASP | A | 113 | 50.478 | 75.882 | 15.230 | 1.00 | 27.64 |
| 1395 | O | ASP | A | 113 | 50.693 | 75.218 | 16.248 | 1.00 | 26.98 |
| 1396 | N | ASP | A | 114 | 49.334 | 75.823 | 14.559 | 1.00 | 26.95 |
| 1398 | CA | ASP | A | 114 | 48.242 | 74.989 | 15.031 | 1.00 | 26.81 |
| 1400 | CB | ASP | A | 114 | 46.929 | 75.778 | 15.089 | 1.00 | 27.66 |
| 1403 | CG | ASP | A | 114 | 46.453 | 76.241 | 13.725 | 1.00 | 30.37 |
| 1404 | OD1 | ASP | A | 114 | 45.282 | 76.700 | 13.645 | 1.00 | 33.61 |
| 1405 | OD2 | ASP | A | 114 | 47.165 | 76.194 | 12.690 | 1.00 | 32.04 |
| 1406 | C | ASP | A | 114 | 48.075 | 73.702 | 14.236 | 1.00 | 25.96 |
| 1407 | O | ASP | A | 114 | 47.283 | 72.856 | 14.631 | 1.00 | 25.76 |
| 1408 | N | LEU | A | 115 | 48.818 | 73.559 | 13.136 | 1.00 | 25.04 |
| 1410 | CA | LEU | A | 115 | 48.751 | 72.367 | 12.298 | 1.00 | 24.85 |
| 1412 | CB | LEU | A | 115 | 48.106 | 72.694 | 10.945 | 1.00 | 25.33 |
| 1415 | CG | LEU | A | 115 | 46.598 | 72.821 | 10.810 | 1.00 | 26.83 |
| 1417 | CD1 | LEU | A | 115 | 46.260 | 73.283 | 9.399 | 1.00 | 29.44 |
| 1421 | CD2 | LEU | A | 115 | 45.903 | 71.492 | 11.089 | 1.00 | 27.95 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 1425 | C | LEU | A | 115 | 50.144 | 71.781 | 12.034 | 1.00 | 23.64 |
| 1426 | O | LEU | A | 115 | 51.094 | 72.514 | 11.790 | 1.00 | 23.64 |
| 1427 | N | ARG | A | 116 | 50.237 | 70.454 | 12.081 | 1.00 | 22.79 |
| 1429 | CA | ARG | A | 116 | 51.401 | 69.715 | 11.603 | 1.00 | 22.20 |
| 1431 | CB | ARG | A | 116 | 52.479 | 69.644 | 12.672 | 1.00 | 21.90 |
| 1434 | CG | ARG | A | 116 | 53.742 | 69.015 | 12.166 | 1.00 | 21.62 |
| 1437 | CD | ARG | A | 116 | 54.820 | 68.975 | 13.195 | 1.00 | 21.16 |
| 1440 | NE | ARG | A | 116 | 55.377 | 70.290 | 13.472 | 1.00 | 19.55 |
| 1442 | CZ | ARG | A | 116 | 56.277 | 70.905 | 12.721 | 1.00 | 21.19 |
| 1443 | NH1 | ARG | A | 116 | 56.740 | 72.082 | 13.111 | 1.00 | 21.55 |
| 1446 | NH2 | ARG | A | 116 | 56.737 | 70.355 | 11.590 | 1.00 | 21.98 |
| 1449 | C | ARG | A | 116 | 50.997 | 68.301 | 11.215 | 1.00 | 21.87 |
| 1450 | O | ARG | A | 116 | 50.184 | 67.686 | 11.876 | 1.00 | 20.97 |
| 1451 | N | ARG | A | 117 | 51.566 | 67.807 | 10.122 | 1.00 | 22.79 |
| 1453 | CA | ARG | A | 117 | 51.237 | 66.489 | 9.580 | 1.00 | 23.42 |
| 1455 | CB | ARG | A | 117 | 51.814 | 65.407 | 10.477 | 1.00 | 23.33 |
| 1458 | CG | ARG | A | 117 | 53.310 | 65.424 | 10.531 | 1.00 | 22.10 |
| 1461 | CD | ARG | A | 117 | 53.841 | 64.752 | 11.768 | 1.00 | 21.59 |
| 1464 | NE | ARG | A | 117 | 55.282 | 64.632 | 11.726 | 1.00 | 21.10 |
| 1466 | CZ | ARG | A | 117 | 56.009 | 64.082 | 12.681 | 1.00 | 21.03 |
| 1467 | NH1 | ARG | A | 117 | 55.438 | 63.576 | 13.760 | 1.00 | 20.75 |
| 1470 | NH2 | ARG | A | 117 | 57.323 | 64.020 | 12.544 | 1.00 | 22.79 |
| 1473 | C | ARG | A | 117 | 49.733 | 66.284 | 9.374 | 1.00 | 24.49 |
| 1474 | O | ARG | A | 117 | 49.216 | 65.181 | 9.528 | 1.00 | 24.90 |
| 1475 | N | GLY | A | 118 | 49.048 | 67.375 | 9.037 | 1.00 | 25.84 |
| 1477 | CA | GLY | A | 118 | 47.641 | 67.363 | 8.673 | 1.00 | 26.45 |
| 1480 | C | GLY | A | 118 | 46.709 | 67.432 | 9.854 | 1.00 | 27.01 |
| 1481 | O | GLY | A | 118 | 45.500 | 67.383 | 9.663 | 1.00 | 27.66 |
| 1482 | N | LEU | A | 119 | 47.258 | 67.574 | 11.066 | 1.00 | 27.18 |
| 1484 | CA | LEU | A | 119 | 46.478 | 67.445 | 12.301 | 1.00 | 27.29 |
| 1486 | CB | LEU | A | 119 | 46.778 | 66.104 | 12.965 | 1.00 | 27.61 |
| 1489 | CG | LEU | A | 119 | 46.308 | 64.849 | 12.230 | 1.00 | 29.25 |
| 1491 | CD1 | LEU | A | 119 | 46.956 | 63.639 | 12.826 | 1.00 | 29.40 |
| 1495 | CD2 | LEU | A | 119 | 44.799 | 64.723 | 12.297 | 1.00 | 30.33 |
| 1499 | C | LEU | A | 119 | 46.783 | 68.580 | 13.279 | 1.00 | 26.95 |
| 1500 | O | LEU | A | 119 | 47.781 | 69.273 | 13.134 | 1.00 | 26.97 |
| 1501 | N | PRO | A | 120 | 45.911 | 68.807 | 14.256 | 1.00 | 26.77 |
| 1502 | CA | PRO | A | 120 | 46.242 | 69.737 | 15.341 | 1.00 | 26.42 |
| 1504 | CB | PRO | A | 120 | 45.151 | 69.465 | 16.391 | 1.00 | 26.39 |
| 1507 | CG | PRO | A | 120 | 43.997 | 68.927 | 15.636 | 1.00 | 27.10 |
| 1510 | CD | PRO | A | 120 | 44.540 | 68.278 | 14.377 | 1.00 | 27.03 |
| 1513 | C | PRO | A | 120 | 47.644 | 69.428 | 15.902 | 1.00 | 25.96 |
| 1514 | O | PRO | A | 120 | 47.988 | 68.247 | 16.088 | 1.00 | 25.12 |
| 1515 | N | THR | A | 121 | 48.433 | 70.470 | 16.131 | 1.00 | 25.63 |
| 1517 | CA | THR | A | 121 | 49.730 | 70.336 | 16.803 | 1.00 | 25.53 |
| 1519 | CB | THR | A | 121 | 50.478 | 71.668 | 16.835 | 1.00 | 25.67 |
| 1521 | OG1 | THR | A | 121 | 49.605 | 72.715 | 17.288 | 1.00 | 26.41 |
| 1523 | CG2 | THR | A | 121 | 50.901 | 72.085 | 15.442 | 1.00 | 25.77 |
| 1527 | C | THR | A | 121 | 49.531 | 69.838 | 18.228 | 1.00 | 25.27 |
| 1528 | O | THR | A | 121 | 48.430 | 69.941 | 18.787 | 1.00 | 24.78 |
| 1529 | N | CYS | A | 122 | 50.600 | 69.305 | 18.817 | 1.00 | 24.89 |
| 1531 | CA | CYS | A | 122 | 50.523 | 68.697 | 20.137 | 1.00 | 24.95 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 1533 | CB | CYS | A | 122 | 51.895 | 68.165 | 20.581 | 1.00 | 24.90 |
| 1536 | SG | CYS | A | 122 | 52.285 | 66.565 | 19.821 | 1.00 | 24.91 |
| 1537 | C | CYS | A | 122 | 49.933 | 69.634 | 21.182 | 1.00 | 24.97 |
| 1538 | O | CYS | A | 122 | 49.096 | 69.228 | 21.971 | 1.00 | 24.71 |
| 1539 | N | HIS | A | 123 | 50.346 | 70.894 | 21.168 | 1.00 | 25.78 |
| 1541 | CA | HIS | A | 123 | 49.925 | 71.820 | 22.208 | 1.00 | 26.16 |
| 1543 | CB | HIS | A | 123 | 50.836 | 73.054 | 22.246 | 1.00 | 26.51 |
| 1546 | CG | HIS | A | 123 | 50.548 | 74.067 | 21.186 | 1.00 | 27.10 |
| 1547 | ND1 | HIS | A | 123 | 50.785 | 73.840 | 19.849 | 1.00 | 30.89 |
| 1549 | CE1 | HIS | A | 123 | 50.441 | 74.911 | 19.156 | 1.00 | 30.52 |
| 1551 | NE2 | HIS | A | 123 | 50.007 | 75.831 | 19.996 | 1.00 | 30.35 |
| 1553 | CD2 | HIS | A | 123 | 50.066 | 75.327 | 21.272 | 1.00 | 29.44 |
| 1555 | C | HIS | A | 123 | 48.433 | 72.162 | 22.054 | 1.00 | 26.69 |
| 1556 | O | HIS | A | 123 | 47.747 | 72.385 | 23.040 | 1.00 | 26.52 |
| 1557 | N | VAL | A | 124 | 47.938 | 72.180 | 20.820 | 1.00 | 27.17 |
| 1559 | CA | VAL | A | 124 | 46.510 | 72.380 | 20.577 | 1.00 | 27.86 |
| 1561 | CB | VAL | A | 124 | 46.217 | 72.617 | 19.078 | 1.00 | 27.70 |
| 1563 | CG1 | VAL | A | 124 | 44.701 | 72.510 | 18.774 | 1.00 | 28.86 |
| 1567 | CG2 | VAL | A | 124 | 46.737 | 73.972 | 18.645 | 1.00 | 28.14 |
| 1571 | C | VAL | A | 124 | 45.695 | 71.196 | 21.131 | 1.00 | 28.24 |
| 1572 | O | VAL | A | 124 | 44.784 | 71.396 | 21.935 | 1.00 | 28.47 |
| 1573 | N | LYS | A | 125 | 46.040 | 69.973 | 20.733 | 1.00 | 28.54 |
| 1575 | CA | LYS | A | 125 | 45.245 | 68.798 | 21.101 | 1.00 | 29.34 |
| 1577 | CB | LYS | A | 125 | 45.617 | 67.583 | 20.241 | 1.00 | 29.61 |
| 1580 | CG | LYS | A | 125 | 44.863 | 66.301 | 20.626 | 1.00 | 30.82 |
| 1583 | CD | LYS | A | 125 | 45.106 | 65.186 | 19.627 | 1.00 | 32.53 |
| 1586 | CE | LYS | A | 125 | 44.199 | 63.976 | 19.839 | 1.00 | 33.76 |
| 1589 | NZ | LYS | A | 125 | 43.344 | 64.050 | 21.054 | 1.00 | 36.05 |
| 1593 | C | LYS | A | 125 | 45.371 | 68.422 | 22.581 | 1.00 | 29.59 |
| 1594 | O | LYS | A | 125 | 44.383 | 68.012 | 23.194 | 1.00 | 29.82 |
| 1595 | N | PHE | A | 126 | 46.575 | 68.551 | 23.146 | 1.00 | 28.84 |
| 1597 | CA | PHE | A | 126 | 46.839 | 68.108 | 24.519 | 1.00 | 28.62 |
| 1599 | CB | PHE | A | 126 | 47.984 | 67.096 | 24.529 | 1.00 | 28.31 |
| 1602 | CG | PHE | A | 126 | 47.722 | 65.880 | 23.711 | 1.00 | 27.28 |
| 1603 | CD1 | PHE | A | 126 | 47.055 | 64.787 | 24.261 | 1.00 | 27.38 |
| 1605 | CE1 | PHE | A | 126 | 46.831 | 63.631 | 23.508 | 1.00 | 27.16 |
| 1607 | CZ | PHE | A | 126 | 47.271 | 63.563 | 22.198 | 1.00 | 27.58 |
| 1609 | CE2 | PHE | A | 126 | 47.932 | 64.648 | 21.636 | 1.00 | 27.23 |
| 1611 | CD2 | PHE | A | 126 | 48.163 | 65.804 | 22.399 | 1.00 | 27.44 |
| 1613 | C | PHE | A | 126 | 47.185 | 69.217 | 25.515 | 1.00 | 28.26 |
| 1614 | O | PHE | A | 126 | 47.341 | 68.943 | 26.706 | 1.00 | 29.25 |
| 1615 | N | GLY | A | 127 | 47.299 | 70.452 | 25.042 | 1.00 | 27.60 |
| 1617 | CA | GLY | A | 127 | 47.659 | 71.575 | 25.896 | 1.00 | 26.94 |
| 1620 | C | GLY | A | 127 | 49.155 | 71.840 | 25.860 | 1.00 | 26.46 |
| 1621 | O | GLY | A | 127 | 49.958 | 70.992 | 25.438 | 1.00 | 26.06 |
| 1622 | N | GLU | A | 128 | 49.536 | 73.009 | 26.340 | 1.00 | 25.72 |
| 1624 | CA | GLU | A | 128 | 50.910 | 73.462 | 26.248 | 1.00 | 25.58 |
| 1626 | CB | GLU | A | 128 | 51.007 | 74.958 | 26.519 | 1.00 | 25.87 |
| 1629 | CG | GLU | A | 128 | 50.483 | 75.783 | 25.358 | 1.00 | 29.11 |
| 1632 | CD | GLU | A | 128 | 50.355 | 77.241 | 25.698 | 1.00 | 33.26 |
| 1633 | OE1 | GLU | A | 128 | 51.247 | 77.754 | 26.399 | 1.00 | 35.51 |
| 1634 | OE2 | GLU | A | 128 | 49.349 | 77.861 | 25.269 | 1.00 | 37.97 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 1635 | C | GLU | A | 128 | 51.798 | 72.689 | 27.211 | 1.00 | 24.80 |
| 1636 | O | GLU | A | 128 | 52.899 | 72.300 | 26.840 | 1.00 | 24.40 |
| 1637 | N | ALA | A | 129 | 51.320 | 72.474 | 28.436 | 1.00 | 23.77 |
| 1639 | CA | ALA | A | 129 | 52.098 | 71.760 | 29.447 | 1.00 | 23.73 |
| 1641 | CB | ALA | A | 129 | 51.353 | 71.711 | 30.776 | 1.00 | 23.98 |
| 1645 | C | ALA | A | 129 | 52.441 | 70.343 | 28.968 | 1.00 | 23.81 |
| 1646 | O | ALA | A | 129 | 53.603 | 69.943 | 29.024 | 1.00 | 24.19 |
| 1647 | N | ASN | A | 130 | 51.442 | 69.609 | 28.479 | 1.00 | 22.86 |
| 1649 | CA | ASN | A | 130 | 51.654 | 68.270 | 27.947 | 1.00 | 22.86 |
| 1651 | CB | ASN | A | 130 | 50.345 | 67.623 | 27.491 | 1.00 | 23.02 |
| 1654 | CG | ASN | A | 130 | 49.539 | 67.041 | 28.635 | 1.00 | 24.68 |
| 1655 | OD1 | ASN | A | 130 | 48.304 | 67.110 | 28.640 | 1.00 | 27.85 |
| 1656 | ND2 | ASN | A | 130 | 50.220 | 66.461 | 29.600 | 1.00 | 25.67 |
| 1659 | C | ASN | A | 130 | 52.631 | 68.261 | 26.779 | 1.00 | 21.84 |
| 1660 | O | ASN | A | 130 | 53.428 | 67.339 | 26.667 | 1.00 | 22.15 |
| 1661 | N | ALA | A | 131 | 52.543 | 69.263 | 25.908 | 1.00 | 20.33 |
| 1663 | CA | ALA | A | 131 | 53.457 | 69.399 | 24.788 | 1.00 | 20.39 |
| 1665 | CB | ALA | A | 131 | 52.984 | 70.529 | 23.886 | 1.00 | 20.63 |
| 1669 | C | ALA | A | 131 | 54.925 | 69.621 | 25.250 | 1.00 | 19.95 |
| 1670 | O | ALA | A | 131 | 55.856 | 68.974 | 24.760 | 1.00 | 19.97 |
| 1671 | N | ILE | A | 132 | 55.117 | 70.509 | 26.218 | 1.00 | 19.41 |
| 1673 | CA | ILE | A | 132 | 56.434 | 70.769 | 26.790 | 1.00 | 19.39 |
| 1675 | CB | ILE | A | 132 | 56.357 | 71.842 | 27.880 | 1.00 | 19.07 |
| 1677 | CG1 | ILE | A | 132 | 56.032 | 73.214 | 27.267 | 1.00 | 20.58 |
| 1680 | CD1 | ILE | A | 132 | 55.450 | 74.180 | 28.244 | 1.00 | 22.11 |
| 1684 | CG2 | ILE | A | 132 | 57.668 | 71.944 | 28.623 | 1.00 | 19.77 |
| 1688 | C | ILE | A | 132 | 57.011 | 69.487 | 27.378 | 1.00 | 19.19 |
| 1689 | O | ILE | A | 132 | 58.134 | 69.105 | 27.069 | 1.00 | 18.97 |
| 1690 | N | LEU | A | 133 | 56.229 | 68.824 | 28.211 | 1.00 | 18.52 |
| 1692 | CA | LEU | A | 133 | 56.694 | 67.637 | 28.913 | 1.00 | 19.19 |
| 1694 | CB | LEU | A | 133 | 55.716 | 67.252 | 30.029 | 1.00 | 19.06 |
| 1697 | CG | LEU | A | 133 | 55.616 | 68.280 | 31.166 | 1.00 | 20.37 |
| 1699 | CD1 | LEU | A | 133 | 56.961 | 68.500 | 31.859 | 1.00 | 22.60 |
| 1703 | CD2 | LEU | A | 133 | 54.595 | 67.820 | 32.159 | 1.00 | 21.48 |
| 1707 | C | LEU | A | 133 | 56.907 | 66.470 | 27.966 | 1.00 | 18.53 |
| 1708 | O | LEU | A | 133 | 57.856 | 65.723 | 28.126 | 1.00 | 18.41 |
| 1709 | N | ALA | A | 134 | 56.033 | 66.320 | 26.973 | 1.00 | 17.92 |
| 1711 | CA | ALA | A | 134 | 56.179 | 65.228 | 26.012 | 1.00 | 17.62 |
| 1713 | CB | ALA | A | 134 | 54.947 | 65.115 | 25.104 | 1.00 | 17.67 |
| 1717 | C | ALA | A | 134 | 57.434 | 65.418 | 25.168 | 1.00 | 17.09 |
| 1718 | O | ALA | A | 134 | 58.108 | 64.461 | 24.828 | 1.00 | 17.12 |
| 1719 | N | GLY | A | 135 | 57.740 | 66.649 | 24.807 | 1.00 | 16.81 |
| 1721 | CA | GLY | A | 135 | 58.945 | 66.914 | 24.059 | 1.00 | 16.96 |
| 1724 | C | GLY | A | 135 | 60.155 | 66.651 | 24.946 | 1.00 | 17.30 |
| 1725 | O | GLY | A | 135 | 61.102 | 66.022 | 24.500 | 1.00 | 17.59 |
| 1726 | N | ASP | A | 136 | 60.106 | 67.121 | 26.193 | 1.00 | 17.16 |
| 1728 | CA | ASP | A | 136 | 61.139 | 66.853 | 27.190 | 1.00 | 17.77 |
| 1730 | CB | ASP | A | 136 | 60.717 | 67.383 | 28.562 | 1.00 | 18.20 |
| 1733 | CG | ASP | A | 136 | 60.801 | 68.881 | 28.661 | 1.00 | 19.18 |
| 1734 | OD1 | ASP | A | 136 | 61.407 | 69.492 | 27.759 | 1.00 | 21.99 |
| 1735 | OD2 | ASP | A | 136 | 60.295 | 69.527 | 29.612 | 1.00 | 19.91 |
| 1736 | C | ASP | A | 136 | 61.410 | 65.359 | 27.301 | 1.00 | 17.64 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 1737 | O | ASP | A | 136 | 62.548 | 64.927 | 27.230 | 1.00 | 17.90 |
| 1738 | N | ALA | A | 137 | 60.343 | 64.584 | 27.447 | 1.00 | 17.42 |
| 1740 | CA | ALA | A | 137 | 60.438 | 63.146 | 27.633 | 1.00 | 17.39 |
| 1742 | CB | ALA | A | 137 | 59.098 | 62.582 | 28.089 | 1.00 | 17.97 |
| 1746 | C | ALA | A | 137 | 60.910 | 62.429 | 26.378 | 1.00 | 17.06 |
| 1747 | O | ALA | A | 137 | 61.576 | 61.425 | 26.482 | 1.00 | 16.51 |
| 1748 | N | LEU | A | 138 | 60.525 | 62.918 | 25.197 | 1.00 | 17.23 |
| 1750 | CA | LEU | A | 138 | 61.005 | 62.333 | 23.947 | 1.00 | 17.60 |
| 1752 | CB | LEU | A | 138 | 60.265 | 62.904 | 22.740 | 1.00 | 17.59 |
| 1755 | CG | LEU | A | 138 | 58.930 | 62.247 | 22.427 | 1.00 | 17.08 |
| 1757 | CD1 | LEU | A | 138 | 58.170 | 63.044 | 21.399 | 1.00 | 18.87 |
| 1761 | CD2 | LEU | A | 138 | 59.126 | 60.798 | 21.970 | 1.00 | 18.78 |
| 1765 | C | LEU | A | 138 | 62.515 | 62.534 | 23.779 | 1.00 | 17.74 |
| 1766 | O | LEU | A | 138 | 63.197 | 61.641 | 23.297 | 1.00 | 17.61 |
| 1767 | N | GLN | A | 139 | 63.036 | 63.695 | 24.185 | 1.00 | 17.96 |
| 1769 | CA | GLN | A | 139 | 64.483 | 63.926 | 24.148 | 1.00 | 18.23 |
| 1771 | CB | GLN | A | 139 | 64.894 | 65.366 | 24.559 | 1.00 | 18.28 |
| 1774 | CG | GLN | A | 139 | 66.427 | 65.512 | 24.520 | 1.00 | 19.50 |
| 1777 | CD | GLN | A | 139 | 67.021 | 66.816 | 25.074 | 1.00 | 22.38 |
| 1778 | OE1 | GLN | A | 139 | 66.350 | 67.833 | 25.237 | 1.00 | 19.65 |
| 1779 | NE2 | GLN | A | 139 | 68.322 | 66.768 | 25.346 | 1.00 | 23.26 |
| 1782 | C | GLN | A | 139 | 65.165 | 62.906 | 25.043 | 1.00 | 17.62 |
| 1783 | O | GLN | A | 139 | 66.132 | 62.284 | 24.645 | 1.00 | 17.06 |
| 1784 | N | THR | A | 140 | 64.650 | 62.736 | 26.258 | 1.00 | 18.05 |
| 1786 | CA | THR | A | 140 | 65.220 | 61.790 | 27.201 | 1.00 | 18.07 |
| 1788 | CB | THR | A | 140 | 64.461 | 61.797 | 28.520 | 1.00 | 18.89 |
| 1790 | OG1 | THR | A | 140 | 64.445 | 63.109 | 29.073 | 1.00 | 17.91 |
| 1792 | CG2 | THR | A | 140 | 65.189 | 60.940 | 29.551 | 1.00 | 18.65 |
| 1796 | C | THR | A | 140 | 65.165 | 60.373 | 26.665 | 1.00 | 17.74 |
| 1797 | O | THR | A | 140 | 66.111 | 59.615 | 26.829 | 1.00 | 17.70 |
| 1798 | N | LEU | A | 141 | 64.056 | 60.037 | 26.016 | 1.00 | 17.32 |
| 1800 | CA | LEU | A | 141 | 63.863 | 58.698 | 25.487 | 1.00 | 17.21 |
| 1802 | CB | LEU | A | 141 | 62.450 | 58.554 | 24.899 | 1.00 | 16.68 |
| 1805 | CG | LEU | A | 141 | 62.102 | 57.160 | 24.360 | 1.00 | 17.14 |
| 1807 | CD1 | LEU | A | 141 | 62.252 | 56.096 | 25.413 | 1.00 | 17.24 |
| 1811 | CD2 | LEU | A | 141 | 60.691 | 57.141 | 23.772 | 1.00 | 17.71 |
| 1815 | C | LEU | A | 141 | 64.934 | 58.362 | 24.443 | 1.00 | 16.99 |
| 1816 | O | LEU | A | 141 | 65.396 | 57.234 | 24.373 | 1.00 | 17.51 |
| 1817 | N | ALA | A | 142 | 65.311 | 59.345 | 23.637 | 1.00 | 16.86 |
| 1819 | CA | ALA | A | 142 | 66.350 | 59.191 | 22.640 | 1.00 | 16.98 |
| 1821 | CB | ALA | A | 142 | 66.617 | 60.525 | 21.936 | 1.00 | 16.96 |
| 1825 | C | ALA | A | 142 | 67.629 | 58.656 | 23.286 | 1.00 | 17.44 |
| 1826 | O | ALA | A | 142 | 68.269 | 57.772 | 22.741 | 1.00 | 17.77 |
| 1827 | N | PHE | A | 143 | 67.982 | 59.193 | 24.449 | 1.00 | 17.78 |
| 1829 | CA | PHE | A | 143 | 69.179 | 58.770 | 25.172 | 1.00 | 18.09 |
| 1831 | CB | PHE | A | 143 | 69.700 | 59.891 | 26.062 | 1.00 | 18.06 |
| 1834 | CG | PHE | A | 143 | 70.113 | 61.073 | 25.279 | 1.00 | 18.66 |
| 1835 | CD1 | PHE | A | 143 | 69.308 | 62.203 | 25.215 | 1.00 | 17.95 |
| 1837 | CE1 | PHE | A | 143 | 69.672 | 63.284 | 24.422 | 1.00 | 18.78 |
| 1839 | CZ | PHE | A | 143 | 70.834 | 63.241 | 23.689 | 1.00 | 18.81 |
| 1841 | CE2 | PHE | A | 143 | 71.647 | 62.108 | 23.742 | 1.00 | 19.03 |
| 1843 | CD2 | PHE | A | 143 | 71.277 | 61.031 | 24.526 | 1.00 | 19.55 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 1845 | C | PHE | A | 143 | 69.000 | 57.481 | 25.944 | 1.00 | 17.78 |
| 1846 | O | PHE | A | 143 | 69.967 | 56.741 | 26.093 | 1.00 | 19.01 |
| 1847 | N | SER | A | 144 | 67.783 | 57.181 | 26.383 | 1.00 | 17.63 |
| 1849 | CA | SER | A | 144 | 67.480 | 55.853 | 26.930 | 1.00 | 17.81 |
| 1851 | CB | SER | A | 144 | 66.064 | 55.790 | 27.503 | 1.00 | 18.14 |
| 1854 | OG | SER | A | 144 | 65.998 | 56.474 | 28.749 | 1.00 | 19.62 |
| 1856 | C | SER | A | 144 | 67.634 | 54.788 | 25.860 | 1.00 | 17.61 |
| 1857 | O | SER | A | 144 | 68.139 | 53.706 | 26.127 | 1.00 | 17.31 |
| 1858 | N | ILE | A | 145 | 67.202 | 55.100 | 24.646 | 1.00 | 17.34 |
| 1860 | CA | ILE | A | 145 | 67.275 | 54.150 | 23.545 | 1.00 | 18.07 |
| 1862 | CB | ILE | A | 145 | 66.528 | 54.676 | 22.286 | 1.00 | 18.17 |
| 1864 | CG1 | ILE | A | 145 | 65.001 | 54.638 | 22.531 | 1.00 | 18.76 |
| 1867 | CD1 | ILE | A | 145 | 64.188 | 55.429 | 21.499 | 1.00 | 19.79 |
| 1871 | CG2 | ILE | A | 145 | 66.878 | 53.836 | 21.073 | 1.00 | 19.10 |
| 1875 | C | ILE | A | 145 | 68.732 | 53.827 | 23.237 | 1.00 | 17.54 |
| 1876 | O | ILE | A | 145 | 69.102 | 52.663 | 23.207 | 1.00 | 17.29 |
| 1877 | N | LEU | A | 146 | 69.556 | 54.854 | 23.081 | 1.00 | 17.52 |
| 1879 | CA | LEU | A | 146 | 70.961 | 54.677 | 22.710 | 1.00 | 18.26 |
| 1881 | CB | LEU | A | 146 | 71.607 | 56.028 | 22.388 | 1.00 | 18.48 |
| 1884 | CG | LEU | A | 146 | 71.151 | 56.649 | 21.066 | 1.00 | 18.76 |
| 1886 | CD1 | LEU | A | 146 | 71.890 | 57.952 | 20.786 | 1.00 | 19.92 |
| 1890 | CD2 | LEU | A | 146 | 71.349 | 55.663 | 19.939 | 1.00 | 19.54 |
| 1894 | C | LEU | A | 146 | 71.775 | 53.986 | 23.786 | 1.00 | 18.96 |
| 1895 | O | LEU | A | 146 | 72.715 | 53.265 | 23.476 | 1.00 | 18.14 |
| 1896 | N | SER | A | 147 | 71.414 | 54.201 | 25.046 | 1.00 | 19.45 |
| 1898 | CA | SER | A | 147 | 72.165 | 53.596 | 26.142 | 1.00 | 20.52 |
| 1900 | CB | SER | A | 147 | 72.125 | 54.482 | 27.404 | 1.00 | 20.39 |
| 1903 | OG | SER | A | 147 | 70.812 | 54.763 | 27.813 | 1.00 | 22.72 |
| 1905 | C | SER | A | 147 | 71.707 | 52.157 | 26.439 | 1.00 | 20.99 |
| 1906 | O | SER | A | 147 | 72.535 | 51.344 | 26.874 | 1.00 | 21.12 |
| 1907 | N | ASP | A | 148 | 70.435 | 51.840 | 26.157 | 1.00 | 20.94 |
| 1909 | CA | ASP | A | 148 | 69.803 | 50.583 | 26.617 | 1.00 | 21.52 |
| 1911 | CB | ASP | A | 148 | 68.510 | 50.885 | 27.360 | 1.00 | 21.35 |
| 1914 | CG | ASP | A | 148 | 68.740 | 51.573 | 28.668 | 1.00 | 23.16 |
| 1915 | OD1 | ASP | A | 148 | 67.745 | 52.038 | 29.261 | 1.00 | 22.75 |
| 1916 | OD2 | ASP | A | 148 | 69.871 | 51.678 | 29.188 | 1.00 | 24.41 |
| 1917 | C | ASP | A | 148 | 69.436 | 49.569 | 25.557 | 1.00 | 21.65 |
| 1918 | O | ASP | A | 148 | 69.308 | 48.382 | 25.850 | 1.00 | 20.45 |
| 1919 | N | ALA | A | 149 | 69.203 | 50.033 | 24.342 | 1.00 | 22.42 |
| 1921 | CA | ALA | A | 149 | 68.645 | 49.176 | 23.301 | 1.00 | 23.31 |
| 1923 | CB | ALA | A | 149 | 68.113 | 50.004 | 22.165 | 1.00 | 22.74 |
| 1927 | C | ALA | A | 149 | 69.698 | 48.200 | 22.795 | 1.00 | 24.09 |
| 1928 | O | ALA | A | 149 | 70.895 | 48.453 | 22.888 | 1.00 | 24.03 |
| 1929 | N | ASP | A | 150 | 69.228 | 47.087 | 22.256 | 1.00 | 25.84 |
| 1931 | CA | ASP | A | 150 | 70.096 | 46.051 | 21.707 | 1.00 | 27.11 |
| 1933 | CB | ASP | A | 150 | 69.309 | 44.768 | 21.402 | 1.00 | 27.68 |
| 1936 | CG | ASP | A | 150 | 68.293 | 44.426 | 22.469 | 1.00 | 31.56 |
| 1937 | OD1 | ASP | A | 150 | 67.116 | 44.829 | 22.309 | 1.00 | 38.25 |
| 1938 | OD2 | ASP | A | 150 | 68.558 | 43.752 | 23.487 | 1.00 | 35.92 |
| 1939 | C | ASP | A | 150 | 70.716 | 46.563 | 20.420 | 1.00 | 26.94 |
| 1940 | O | ASP | A | 150 | 69.995 | 46.966 | 19.504 | 1.00 | 27.42 |
| 1941 | N | MET | A | 151 | 72.044 | 46.586 | 20.374 | 1.00 | 27.00 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 1943 | CA | MET | A | 151 | 72.794 | 46.828 | 19.148 | 1.00 | 27.40 |
| 1945 | CB | MET | A | 151 | 73.297 | 48.273 | 19.105 | 1.00 | 27.32 |
| 1948 | CG | MET | A | 151 | 72.199 | 49.301 | 19.048 | 1.00 | 27.17 |
| 1951 | SD | MET | A | 151 | 72.806 | 50.970 | 18.731 | 1.00 | 27.97 |
| 1952 | CE | MET | A | 151 | 73.747 | 51.294 | 20.169 | 1.00 | 26.35 |
| 1956 | C | MET | A | 151 | 73.972 | 45.850 | 19.125 | 1.00 | 28.08 |
| 1957 | O | MET | A | 151 | 75.099 | 46.213 | 19.487 | 1.00 | 27.86 |
| 1958 | N | PRO | A | 152 | 73.702 | 44.596 | 18.768 | 1.00 | 28.99 |
| 1959 | CA | PRO | A | 152 | 74.700 | 43.519 | 18.900 | 1.00 | 29.80 |
| 1961 | CB | PRO | A | 152 | 74.018 | 42.301 | 18.244 | 1.00 | 30.17 |
| 1964 | CG | PRO | A | 152 | 72.730 | 42.788 | 17.654 | 1.00 | 29.78 |
| 1967 | CD | PRO | A | 152 | 72.402 | 44.090 | 18.296 | 1.00 | 29.22 |
| 1970 | C | PRO | A | 152 | 76.088 | 43.778 | 18.280 | 1.00 | 29.90 |
| 1971 | O | PRO | A | 152 | 77.081 | 43.394 | 18.874 | 1.00 | 30.77 |
| 1972 | N | GLU | A | 153 | 76.176 | 44.452 | 17.149 | 1.00 | 30.07 |
| 1974 | CA | GLU | A | 153 | 77.488 | 44.605 | 16.495 | 1.00 | 30.29 |
| 1976 | CB | GLU | A | 153 | 77.348 | 44.666 | 14.970 | 1.00 | 30.88 |
| 1979 | CG | GLU | A | 153 | 76.419 | 43.625 | 14.368 | 1.00 | 33.60 |
| 1982 | CD | GLU | A | 153 | 74.996 | 44.126 | 14.226 | 1.00 | 36.03 |
| 1983 | OE1 | GLU | A | 153 | 74.447 | 44.088 | 13.102 | 1.00 | 38.00 |
| 1984 | OE2 | GLU | A | 153 | 74.433 | 44.556 | 15.252 | 1.00 | 37.12 |
| 1985 | C | GLU | A | 153 | 78.224 | 45.857 | 16.976 | 1.00 | 28.68 |
| 1986 | O | GLU | A | 153 | 79.335 | 46.129 | 16.528 | 1.00 | 28.50 |
| 1987 | N | VAL | A | 154 | 77.599 | 46.613 | 17.879 | 1.00 | 26.68 |
| 1989 | CA | VAL | A | 154 | 78.056 | 47.949 | 18.205 | 1.00 | 25.01 |
| 1991 | CB | VAL | A | 154 | 76.886 | 48.966 | 18.244 | 1.00 | 25.12 |
| 1993 | CG1 | VAL | A | 154 | 77.404 | 50.369 | 18.438 | 1.00 | 24.25 |
| 1997 | CG2 | VAL | A | 154 | 76.049 | 48.887 | 16.950 | 1.00 | 24.80 |
| 2001 | C | VAL | A | 154 | 78.819 | 47.927 | 19.526 | 1.00 | 23.84 |
| 2002 | O | VAL | A | 154 | 78.271 | 47.605 | 20.585 | 1.00 | 23.11 |
| 2003 | N | SER | A | 155 | 80.098 | 48.254 | 19.440 | 1.00 | 22.76 |
| 2005 | CA | SER | A | 155 | 80.952 | 48.338 | 20.613 | 1.00 | 22.78 |
| 2007 | CB | SER | A | 155 | 82.404 | 48.597 | 20.186 | 1.00 | 22.49 |
| 2010 | OG | SER | A | 155 | 82.568 | 49.915 | 19.707 | 1.00 | 21.57 |
| 2012 | C | SER | A | 155 | 80.458 | 49.448 | 21.539 | 1.00 | 23.11 |
| 2013 | O | SER | A | 155 | 79.794 | 50.402 | 21.099 | 1.00 | 21.95 |
| 2014 | N | ASP | A | 156 | 80.777 | 49.313 | 22.817 | 1.00 | 23.66 |
| 2016 | CA | ASP | A | 156 | 80.499 | 50.348 | 23.801 | 1.00 | 24.49 |
| 2018 | CB | ASP | A | 156 | 81.010 | 49.930 | 25.172 | 1.00 | 25.14 |
| 2021 | CG | ASP | A | 156 | 80.256 | 48.733 | 25.735 | 1.00 | 27.65 |
| 2022 | OD1 | ASP | A | 156 | 80.719 | 48.186 | 26.762 | 1.00 | 31.30 |
| 2023 | OD2 | ASP | A | 156 | 79.201 | 48.281 | 25.225 | 1.00 | 27.89 |
| 2024 | C | ASP | A | 156 | 81.115 | 51.680 | 23.394 | 1.00 | 24.45 |
| 2025 | O | ASP | A | 156 | 80.499 | 52.725 | 23.568 | 1.00 | 23.41 |
| 2026 | N | ARG | A | 157 | 82.319 | 51.639 | 22.827 | 1.00 | 24.28 |
| 2028 | CA | ARG | A | 157 | 82.973 | 52.844 | 22.355 | 1.00 | 24.79 |
| 2030 | CB | ARG | A | 157 | 84.352 | 52.508 | 21.759 | 1.00 | 26.00 |
| 2033 | CG | ARG | A | 157 | 85.134 | 53.699 | 21.268 | 1.00 | 28.93 |
| 2036 | CD | ARG | A | 157 | 85.432 | 54.712 | 22.350 | 1.00 | 34.80 |
| 2039 | NE | ARG | A | 157 | 84.576 | 55.893 | 22.233 | 1.00 | 38.89 |
| 2041 | CZ | ARG | A | 157 | 84.277 | 56.711 | 23.229 | 1.00 | 42.07 |
| 2042 | NH1 | ARG | A | 157 | 83.494 | 57.756 | 22.989 | 1.00 | 43.97 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 2045 | NH2 | ARG | A | 157 | 84.754 | 56.502 | 24.462 | 1.00 | 42.69 |
| 2048 | C | ARG | A | 157 | 82.119 | 53.534 | 21.303 | 1.00 | 23.63 |
| 2049 | O | ARG | A | 157 | 81.949 | 54.749 | 21.330 | 1.00 | 22.68 |
| 2050 | N | ASP | A | 158 | 81.578 | 52.751 | 20.377 | 1.00 | 22.64 |
| 2052 | CA | ASP | A | 158 | 80.765 | 53.305 | 19.316 | 1.00 | 22.05 |
| 2054 | CB | ASP | A | 158 | 80.695 | 52.351 | 18.126 | 1.00 | 22.68 |
| 2057 | CG | ASP | A | 158 | 82.013 | 52.303 | 17.348 | 1.00 | 24.58 |
| 2058 | OD1 | ASP | A | 158 | 82.780 | 53.285 | 17.412 | 1.00 | 24.51 |
| 2059 | OD2 | ASP | A | 158 | 82.369 | 51.328 | 16.654 | 1.00 | 27.53 |
| 2060 | C | ASP | A | 158 | 79.380 | 53.730 | 19.832 | 1.00 | 20.89 |
| 2061 | O | ASP | A | 158 | 78.829 | 54.703 | 19.348 | 1.00 | 19.41 |
| 2062 | N | ARG | A | 159 | 78.855 | 53.043 | 20.844 | 1.00 | 19.83 |
| 2064 | CA | ARG | A | 159 | 77.577 | 53.435 | 21.459 | 1.00 | 18.66 |
| 2066 | CB | ARG | A | 159 | 77.116 | 52.390 | 22.450 | 1.00 | 18.96 |
| 2069 | CG | ARG | A | 159 | 75.734 | 52.644 | 23.008 | 1.00 | 18.87 |
| 2072 | CD | ARG | A | 159 | 75.377 | 51.687 | 24.112 | 1.00 | 19.73 |
| 2075 | NE | ARG | A | 159 | 75.180 | 50.322 | 23.630 | 1.00 | 20.07 |
| 2077 | CZ | ARG | A | 159 | 73.991 | 49.773 | 23.369 | 1.00 | 22.06 |
| 2078 | NH1 | ARG | A | 159 | 73.929 | 48.516 | 22.949 | 1.00 | 20.83 |
| 2081 | NH2 | ARG | A | 159 | 72.862 | 50.466 | 23.521 | 1.00 | 23.23 |
| 2084 | C | ARG | A | 159 | 77.724 | 54.771 | 22.171 | 1.00 | 18.18 |
| 2085 | O | ARG | A | 159 | 76.842 | 55.612 | 22.081 | 1.00 | 17.20 |
| 2086 | N | ILE | A | 160 | 78.847 | 54.959 | 22.869 | 1.00 | 17.73 |
| 2088 | CA | ILE | A | 160 | 79.141 | 56.223 | 23.542 | 1.00 | 18.41 |
| 2090 | CB | ILE | A | 160 | 80.414 | 56.100 | 24.449 | 1.00 | 18.14 |
| 2092 | CG1 | ILE | A | 160 | 80.092 | 55.249 | 25.684 | 1.00 | 19.24 |
| 2095 | CD1 | ILE | A | 160 | 81.307 | 54.703 | 26.408 | 1.00 | 20.01 |
| 2099 | CG2 | ILE | A | 160 | 80.932 | 57.468 | 24.875 | 1.00 | 19.53 |
| 2103 | C | ILE | A | 160 | 79.277 | 57.343 | 22.505 | 1.00 | 17.74 |
| 2104 | O | ILE | A | 160 | 78.757 | 58.424 | 22.698 | 1.00 | 18.17 |
| 2105 | N | SER | A | 161 | 79.934 | 57.063 | 21.388 | 1.00 | 18.18 |
| 2107 | CA | SER | A | 161 | 80.095 | 58.043 | 20.323 | 1.00 | 18.52 |
| 2109 | CB | SER | A | 161 | 81.020 | 57.511 | 19.236 | 1.00 | 18.63 |
| 2112 | OG | SER | A | 161 | 82.330 | 57.395 | 19.748 | 1.00 | 18.50 |
| 2114 | C | SER | A | 161 | 78.744 | 58.437 | 19.718 | 1.00 | 19.05 |
| 2115 | O | SER | A | 161 | 78.538 | 59.594 | 19.368 | 1.00 | 19.13 |
| 2116 | N | MET | A | 162 | 77.836 | 57.476 | 19.618 | 1.00 | 19.12 |
| 2118 | CA | MET | A | 162 | 76.482 | 57.743 | 19.135 | 1.00 | 19.40 |
| 2120 | CB | MET | A | 162 | 75.674 | 56.461 | 19.063 | 1.00 | 19.56 |
| 2123 | CG | MET | A | 162 | 76.083 | 55.564 | 17.948 | 1.00 | 22.23 |
| 2126 | SD | MET | A | 162 | 74.922 | 54.182 | 17.803 | 1.00 | 28.16 |
| 2127 | CE | MET | A | 162 | 75.814 | 53.241 | 16.666 | 1.00 | 26.77 |
| 2131 | C | MET | A | 162 | 75.746 | 58.693 | 20.039 | 1.00 | 18.61 |
| 2132 | O | MET | A | 162 | 75.101 | 59.609 | 19.567 | 1.00 | 18.79 |
| 2133 | N | ILE | A | 163 | 75.826 | 58.439 | 21.342 | 1.00 | 18.55 |
| 2135 | CA | ILE | A | 163 | 75.194 | 59.281 | 22.349 | 1.00 | 17.91 |
| 2137 | CB | ILE | A | 163 | 75.342 | 58.649 | 23.752 | 1.00 | 17.84 |
| 2139 | CG1 | ILE | A | 163 | 74.511 | 57.360 | 23.840 | 1.00 | 18.27 |
| 2142 | CD1 | ILE | A | 163 | 74.814 | 56.495 | 25.017 | 1.00 | 18.88 |
| 2146 | CG2 | ILE | A | 163 | 74.941 | 59.646 | 24.845 | 1.00 | 17.97 |
| 2150 | C | ILE | A | 163 | 75.804 | 60.685 | 22.313 | 1.00 | 17.61 |
| 2151 | O | ILE | A | 163 | 75.087 | 61.683 | 22.308 | 1.00 | 16.93 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 2152 | N | SER | A | 164 | 77.136 | 60.749 | 22.290 | 1.00 | 17.36 |
| 2154 | CA | SER | A | 164 | 77.856 | 62.012 | 22.247 | 1.00 | 17.24 |
| 2156 | CB | SER | A | 164 | 79.372 | 61.759 | 22.292 | 1.00 | 17.57 |
| 2159 | OG | SER | A | 164 | 80.087 | 62.908 | 21.936 | 1.00 | 16.92 |
| 2161 | C | SER | A | 164 | 77.487 | 62.819 | 21.007 | 1.00 | 17.58 |
| 2162 | O | SER | A | 164 | 77.266 | 64.003 | 21.093 | 1.00 | 17.17 |
| 2163 | N | GLU | A | 165 | 77.408 | 62.163 | 19.856 | 1.00 | 18.38 |
| 2165 | CA | GLU | A | 165 | 77.042 | 62.833 | 18.616 | 1.00 | 18.63 |
| 2167 | CB | GLU | A | 165 | 77.242 | 61.904 | 17.409 | 1.00 | 19.18 |
| 2170 | CG | GLU | A | 165 | 76.518 | 62.361 | 16.145 | 1.00 | 20.77 |
| 2173 | CD | GLU | A | 165 | 76.979 | 63.726 | 15.666 | 1.00 | 23.75 |
| 2174 | OE1 | GLU | A | 165 | 78.105 | 64.141 | 16.022 | 1.00 | 24.45 |
| 2175 | OE2 | GLU | A | 165 | 76.233 | 64.384 | 14.918 | 1.00 | 26.52 |
| 2176 | C | GLU | A | 165 | 75.592 | 63.324 | 18.648 | 1.00 | 18.90 |
| 2177 | O | GLU | A | 165 | 75.311 | 64.455 | 18.224 | 1.00 | 18.41 |
| 2178 | N | LEU | A | 166 | 74.671 | 62.489 | 19.122 | 1.00 | 18.15 |
| 2180 | CA | LEU | A | 166 | 73.274 | 62.921 | 19.169 | 1.00 | 18.98 |
| 2182 | CB | LEU | A | 166 | 72.333 | 61.801 | 19.559 | 1.00 | 19.20 |
| 2185 | CG | LEU | A | 166 | 70.845 | 62.123 | 19.337 | 1.00 | 20.03 |
| 2187 | CD1 | LEU | A | 166 | 70.528 | 62.479 | 17.890 | 1.00 | 20.04 |
| 2191 | CD2 | LEU | A | 166 | 70.015 | 60.977 | 19.795 | 1.00 | 21.02 |
| 2195 | C | LEU | A | 166 | 73.119 | 64.115 | 20.113 | 1.00 | 19.39 |
| 2196 | O | LEU | A | 166 | 72.388 | 65.058 | 19.808 | 1.00 | 19.39 |
| 2197 | N | ALA | A | 167 | 73.832 | 64.078 | 21.234 | 1.00 | 19.92 |
| 2199 | CA | ALA | A | 167 | 73.814 | 65.162 | 22.208 | 1.00 | 20.54 |
| 2201 | CB | ALA | A | 167 | 74.591 | 64.764 | 23.463 | 1.00 | 20.76 |
| 2205 | C | ALA | A | 167 | 74.362 | 66.466 | 21.621 | 1.00 | 20.84 |
| 2206 | O | ALA | A | 167 | 73.690 | 67.496 | 21.678 | 1.00 | 21.05 |
| 2207 | N | SER | A | 168 | 75.554 | 66.431 | 21.027 | 1.00 | 21.51 |
| 2209 | CA | SER | A | 168 | 76.138 | 67.660 | 20.486 | 1.00 | 22.08 |
| 2211 | CB | SER | A | 168 | 77.614 | 67.492 | 20.063 | 1.00 | 22.37 |
| 2214 | OG | SER | A | 168 | 77.809 | 66.365 | 19.248 | 1.00 | 24.18 |
| 2216 | C | SER | A | 168 | 75.286 | 68.207 | 19.336 | 1.00 | 21.42 |
| 2217 | O | SER | A | 168 | 75.142 | 69.415 | 19.197 | 1.00 | 21.65 |
| 2218 | N | ALA | A | 169 | 74.700 | 67.316 | 18.539 | 1.00 | 20.43 |
| 2220 | CA | ALA | A | 169 | 73.906 | 67.716 | 17.379 | 1.00 | 20.07 |
| 2222 | CB | ALA | A | 169 | 73.732 | 66.523 | 16.438 | 1.00 | 20.07 |
| 2226 | C | ALA | A | 169 | 72.537 | 68.265 | 17.768 | 1.00 | 19.77 |
| 2227 | O | ALA | A | 169 | 71.937 | 69.041 | 17.026 | 1.00 | 18.96 |
| 2228 | N | SER | A | 170 | 72.026 | 67.836 | 18.922 | 1.00 | 19.92 |
| 2230 | CA | SER | A | 170 | 70.677 | 68.207 | 19.366 | 1.00 | 19.71 |
| 2232 | CB | SER | A | 170 | 70.061 | 67.027 | 20.112 | 1.00 | 20.08 |
| 2235 | OG | SER | A | 170 | 70.098 | 65.862 | 19.285 | 1.00 | 21.77 |
| 2237 | C | SER | A | 170 | 70.655 | 69.452 | 20.246 | 1.00 | 20.10 |
| 2238 | O | SER | A | 170 | 69.661 | 70.210 | 20.271 | 1.00 | 18.98 |
| 2239 | N | GLY | A | 171 | 71.757 | 69.676 | 20.958 | 1.00 | 19.76 |
| 2241 | CA | GLY | A | 171 | 71.846 | 70.733 | 21.939 | 1.00 | 20.35 |
| 2244 | C | GLY | A | 171 | 72.244 | 72.081 | 21.365 | 1.00 | 20.96 |
| 2245 | O | GLY | A | 171 | 71.982 | 72.393 | 20.203 | 1.00 | 20.86 |
| 2246 | N | ILE | A | 172 | 72.900 | 72.879 | 22.200 | 1.00 | 21.84 |
| 2248 | CA | ILE | A | 172 | 73.170 | 74.280 | 21.914 | 1.00 | 22.71 |
| 2250 | CB | ILE | A | 172 | 73.611 | 74.975 | 23.242 | 1.00 | 23.10 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 2252 | CG1 | ILE | A | 172 | 73.194 | 76.437 | 23.239 | 1.00 | 23.87 |
| 2255 | CD1 | ILE | A | 172 | 71.710 | 76.610 | 23.444 | 1.00 | 23.14 |
| 2259 | CG2 | ILE | A | 172 | 75.109 | 74.770 | 23.489 | 1.00 | 25.44 |
| 2263 | C | ILE | A | 172 | 74.197 | 74.443 | 20.769 | 1.00 | 22.75 |
| 2264 | O | ILE | A | 172 | 74.206 | 75.456 | 20.057 | 1.00 | 23.12 |
| 2265 | N | ALA | A | 173 | 75.027 | 73.422 | 20.572 | 1.00 | 22.36 |
| 2267 | CA | ALA | A | 173 | 75.954 | 73.367 | 19.451 | 1.00 | 22.62 |
| 2269 | CB | ALA | A | 173 | 77.109 | 72.455 | 19.770 | 1.00 | 22.85 |
| 2273 | C | ALA | A | 173 | 75.285 | 72.916 | 18.152 | 1.00 | 22.34 |
| 2274 | O | ALA | A | 173 | 75.905 | 72.963 | 17.111 | 1.00 | 22.65 |
| 2275 | N | GLY | A | 174 | 74.028 | 72.488 | 18.212 | 1.00 | 21.57 |
| 2277 | CA | GLY | A | 174 | 73.304 | 72.064 | 17.022 | 1.00 | 21.12 |
| 2280 | C | GLY | A | 174 | 71.883 | 72.588 | 16.982 | 1.00 | 20.68 |
| 2281 | O | GLY | A | 174 | 71.665 | 73.785 | 16.956 | 1.00 | 19.79 |
| 2282 | N | MET | A | 175 | 70.914 | 71.682 | 17.005 | 1.00 | 20.95 |
| 2284 | CA | MET | A | 175 | 69.501 | 72.019 | 16.812 | 1.00 | 20.87 |
| 2286 | CB | MET | A | 175 | 68.655 | 70.757 | 16.927 | 1.00 | 21.21 |
| 2289 | CG | MET | A | 175 | 67.183 | 70.922 | 16.531 | 1.00 | 22.91 |
| 2292 | SD | MET | A | 175 | 66.208 | 71.479 | 17.897 | 1.00 | 28.34 |
| 2293 | CE | MET | A | 175 | 66.254 | 69.967 | 19.003 | 1.00 | 25.97 |
| 2297 | C | MET | A | 175 | 68.952 | 73.140 | 17.721 | 1.00 | 20.52 |
| 2298 | O | MET | A | 175 | 68.310 | 74.072 | 17.224 | 1.00 | 19.77 |
| 2299 | N | CYS | A | 176 | 69.200 | 73.059 | 19.028 | 1.00 | 20.60 |
| 2301 | CA | CYS | A | 176 | 68.689 | 74.061 | 19.977 | 1.00 | 20.42 |
| 2303 | CB | BCYS | A | 176 | 68.958 | 73.590 | 21.405 | 0.35 | 20.62 |
| 2304 | CB | ACYS | A | 176 | 68.958 | 73.668 | 21.427 | 0.65 | 20.89 |
| 2309 | SG | BCYS | A | 176 | 67.803 | 74.234 | 22.609 | 0.35 | 20.91 |
| 2310 | SG | ACYS | A | 176 | 67.804 | 72.489 | 22.098 | 0.65 | 22.71 |
| 2311 | C | CYS | A | 176 | 69.332 | 75.426 | 19.744 | 1.00 | 20.33 |
| 2312 | O | CYS | A | 176 | 68.665 | 76.459 | 19.811 | 1.00 | 18.74 |
| 2313 | N | GLY | A | 177 | 70.650 | 75.414 | 19.539 | 1.00 | 20.11 |
| 2315 | CA | GLY | A | 177 | 71.384 | 76.605 | 19.172 | 1.00 | 20.26 |
| 2318 | C | GLY | A | 177 | 70.807 | 77.252 | 17.932 | 1.00 | 20.35 |
| 2319 | O | GLY | A | 177 | 70.645 | 78.473 | 17.877 | 1.00 | 19.82 |
| 2320 | N | GLY | A | 178 | 70.470 | 76.425 | 16.948 | 1.00 | 20.20 |
| 2322 | CA | GLY | A | 178 | 69.875 | 76.891 | 15.715 | 1.00 | 20.43 |
| 2325 | C | GLY | A | 178 | 68.484 | 77.441 | 15.920 | 1.00 | 20.51 |
| 2326 | O | GLY | A | 178 | 68.117 | 78.435 | 15.303 | 1.00 | 20.93 |
| 2327 | N | GLN | A | 179 | 67.716 | 76.816 | 16.800 | 1.00 | 20.70 |
| 2329 | CA | GLN | A | 179 | 66.397 | 77.327 | 17.168 | 1.00 | 21.15 |
| 2331 | CB | GLN | A | 179 | 65.684 | 76.383 | 18.149 | 1.00 | 21.47 |
| 2334 | CG | GLN | A | 179 | 65.165 | 75.072 | 17.546 | 1.00 | 21.62 |
| 2337 | CD | GLN | A | 179 | 64.102 | 75.279 | 16.494 | 1.00 | 22.97 |
| 2338 | OE1 | GLN | A | 179 | 64.417 | 75.656 | 15.362 | 1.00 | 27.11 |
| 2339 | NE2 | GLN | A | 179 | 62.845 | 75.031 | 16.850 | 1.00 | 22.24 |
| 2342 | C | GLN | A | 179 | 66.514 | 78.725 | 17.794 | 1.00 | 21.59 |
| 2343 | O | GLN | A | 179 | 65.695 | 79.609 | 17.513 | 1.00 | 22.14 |
| 2344 | N | ALA | A | 180 | 67.532 | 78.931 | 18.622 | 1.00 | 21.59 |
| 2346 | CA | ALA | A | 180 | 67.766 | 80.245 | 19.230 | 1.00 | 21.99 |
| 2348 | CB | ALA | A | 180 | 68.847 | 80.166 | 20.296 | 1.00 | 22.20 |
| 2352 | C | ALA | A | 180 | 68.152 | 81.269 | 18.164 | 1.00 | 22.07 |
| 2353 | O | ALA | A | 180 | 67.683 | 82.380 | 18.206 | 1.00 | 21.87 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 2354 | N | LEU | A | 181 | 69.001 | 80.885 | 17.212 | 1.00 | 22.13 |
| 2356 | CA | LEU | A | 181 | 69.369 | 81.776 | 16.106 | 1.00 | 23.00 |
| 2358 | CB | LEU | A | 181 | 70.449 | 81.144 | 15.233 | 1.00 | 23.09 |
| 2361 | CG | LEU | A | 181 | 71.824 | 80.871 | 15.840 | 1.00 | 22.66 |
| 2363 | CD1 | LEU | A | 181 | 72.668 | 80.085 | 14.817 | 1.00 | 24.29 |
| 2367 | CD2 | LEU | A | 181 | 72.522 | 82.155 | 16.235 | 1.00 | 22.45 |
| 2371 | C | LEU | A | 181 | 68.163 | 82.119 | 15.240 | 1.00 | 23.28 |
| 2372 | O | LEU | A | 181 | 68.003 | 83.265 | 14.805 | 1.00 | 23.62 |
| 2373 | N | ASP | A | 182 | 67.314 | 81.123 | 15.002 | 1.00 | 23.53 |
| 2375 | CA | ASP | A | 182 | 66.112 | 81.280 | 14.197 | 1.00 | 24.49 |
| 2377 | CB | ASP | A | 182 | 65.382 | 79.934 | 14.080 | 1.00 | 24.90 |
| 2380 | CG | ASP | A | 182 | 64.004 | 80.064 | 13.491 | 1.00 | 25.57 |
| 2381 | OD1 | ASP | A | 182 | 63.830 | 79.750 | 12.287 | 1.00 | 28.64 |
| 2382 | OD2 | ASP | A | 182 | 63.023 | 80.441 | 14.162 | 1.00 | 28.54 |
| 2383 | C | ASP | A | 182 | 65.187 | 82.320 | 14.841 | 1.00 | 24.97 |
| 2384 | O | ASP | A | 182 | 64.683 | 83.222 | 14.178 | 1.00 | 24.47 |
| 2385 | N | LEU | A | 183 | 64.974 | 82.168 | 16.138 | 1.00 | 25.23 |
| 2387 | CA | LEU | A | 183 | 64.127 | 83.083 | 16.905 | 1.00 | 26.68 |
| 2389 | CB | LEU | A | 183 | 63.977 | 82.575 | 18.343 | 1.00 | 26.78 |
| 2392 | CG | LEU | A | 183 | 62.658 | 81.902 | 18.734 | 1.00 | 28.22 |
| 2394 | CD1 | LEU | A | 183 | 62.016 | 81.077 | 17.633 | 1.00 | 29.14 |
| 2398 | CD2 | LEU | A | 183 | 62.892 | 81.055 | 19.970 | 1.00 | 29.13 |
| 2402 | C | LEU | A | 183 | 64.686 | 84.512 | 16.914 | 1.00 | 26.76 |
| 2403 | O | LEU | A | 183 | 63.936 | 85.474 | 16.784 | 1.00 | 26.89 |
| 2404 | N | ASP | A | 184 | 66.002 | 84.640 | 17.050 | 1.00 | 27.40 |
| 2406 | CA | ASP | A | 184 | 66.636 | 85.952 | 17.078 | 1.00 | 28.30 |
| 2408 | CB | ASP | A | 184 | 68.107 | 85.827 | 17.459 | 1.00 | 28.53 |
| 2411 | CG | ASP | A | 184 | 68.753 | 87.176 | 17.720 | 1.00 | 31.35 |
| 2412 | OD1 | ASP | A | 184 | 69.682 | 87.571 | 16.965 | 1.00 | 33.39 |
| 2413 | OD2 | ASP | A | 184 | 68.389 | 87.907 | 18.667 | 1.00 | 33.95 |
| 2414 | C | ASP | A | 184 | 66.513 | 86.681 | 15.734 | 1.00 | 28.03 |
| 2415 | O | ASP | A | 184 | 66.398 | 87.907 | 15.689 | 1.00 | 27.69 |
| 2416 | N | ALA | A | 185 | 66.525 | 85.915 | 14.648 | 1.00 | 27.46 |
| 2418 | CA | ALA | A | 185 | 66.499 | 86.467 | 13.300 | 1.00 | 27.69 |
| 2420 | CB | ALA | A | 185 | 67.174 | 85.479 | 12.330 | 1.00 | 27.70 |
| 2424 | C | ALA | A | 185 | 65.089 | 86.843 | 12.796 | 1.00 | 27.58 |
| 2425 | O | ALA | A | 185 | 64.946 | 87.351 | 11.683 | 1.00 | 27.80 |
| 2426 | N | GLU | A | 186 | 64.057 | 86.590 | 13.596 | 1.00 | 27.88 |
| 2428 | CA | GLU | A | 186 | 62.702 | 87.040 | 13.277 | 1.00 | 28.36 |
| 2430 | CB | GLU | A | 186 | 61.710 | 86.633 | 14.367 | 1.00 | 28.57 |
| 2433 | CG | GLU | A | 186 | 61.415 | 85.151 | 14.422 | 1.00 | 29.97 |
| 2436 | CD | GLU | A | 186 | 60.434 | 84.780 | 15.517 | 1.00 | 32.47 |
| 2437 | OE1 | GLU | A | 186 | 60.070 | 85.661 | 16.338 | 1.00 | 34.93 |
| 2438 | OE2 | GLU | A | 186 | 60.026 | 83.598 | 15.558 | 1.00 | 32.41 |
| 2439 | C | GLU | A | 186 | 62.695 | 88.560 | 13.162 | 1.00 | 28.40 |
| 2440 | O | GLU | A | 186 | 63.140 | 89.252 | 14.075 | 1.00 | 27.70 |
| 2441 | N | GLY | A | 187 | 62.227 | 89.057 | 12.020 | 1.00 | 28.55 |
| 2443 | CA | GLY | A | 187 | 62.105 | 90.477 | 11.766 | 1.00 | 29.05 |
| 2446 | C | GLY | A | 187 | 63.391 | 91.173 | 11.391 | 1.00 | 29.41 |
| 2447 | O | GLY | A | 187 | 63.379 | 92.382 | 11.129 | 1.00 | 30.34 |
| 2448 | N | LYS | A | 188 | 64.501 | 90.437 | 11.353 | 1.00 | 29.52 |
| 2450 | CA | LYS | A | 188 | 65.818 | 91.032 | 11.137 | 1.00 | 29.58 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 2452 | CB | LYS | A | 188 | 66.807 | 90.510 | 12.175 | 1.00 | 30.25 |
| 2455 | CG | LYS | A | 188 | 66.415 | 90.819 | 13.604 | 1.00 | 31.19 |
| 2458 | CD | LYS | A | 188 | 67.528 | 90.474 | 14.569 | 1.00 | 33.42 |
| 2461 | CE | LYS | A | 188 | 67.168 | 90.894 | 16.009 | 1.00 | 34.43 |
| 2464 | NZ | LYS | A | 188 | 65.969 | 90.178 | 16.544 | 1.00 | 36.01 |
| 2468 | C | LYS | A | 188 | 66.375 | 90.797 | 9.730 | 1.00 | 29.61 |
| 2469 | O | LYS | A | 188 | 67.389 | 91.383 | 9.367 | 1.00 | 29.31 |
| 2470 | N | HIS | A | 189 | 65.725 | 89.944 | 8.947 | 1.00 | 29.18 |
| 2472 | CA | HIS | A | 189 | 66.098 | 89.736 | 7.546 | 1.00 | 29.54 |
| 2474 | CB | HIS | A | 189 | 65.574 | 90.895 | 6.688 | 1.00 | 29.50 |
| 2477 | CG | HIS | A | 189 | 64.099 | 91.086 | 6.806 | 1.00 | 29.04 |
| 2478 | ND1 | HIS | A | 189 | 63.217 | 90.679 | 5.835 | 1.00 | 29.33 |
| 2480 | CE1 | HIS | A | 189 | 61.982 | 90.944 | 6.226 | 1.00 | 30.87 |
| 2482 | NE2 | HIS | A | 189 | 62.033 | 91.486 | 7.429 | 1.00 | 30.77 |
| 2484 | CD2 | HIS | A | 189 | 63.346 | 91.580 | 7.816 | 1.00 | 30.69 |
| 2486 | C | HIS | A | 189 | 67.598 | 89.588 | 7.410 | 1.00 | 29.56 |
| 2487 | O | HIS | A | 189 | 68.261 | 90.375 | 6.732 | 1.00 | 29.82 |
| 2488 | N | VAL | A | 190 | 68.136 | 88.569 | 8.067 | 1.00 | 29.52 |
| 2490 | CA | VAL | A | 190 | 69.580 | 88.461 | 8.215 | 1.00 | 29.40 |
| 2492 | CB | VAL | A | 190 | 69.976 | 87.488 | 9.352 | 1.00 | 29.29 |
| 2494 | CG1 | VAL | A | 190 | 69.310 | 87.904 | 10.659 | 1.00 | 29.32 |
| 2498 | CG2 | VAL | A | 190 | 69.645 | 86.033 | 8.998 | 1.00 | 28.66 |
| 2502 | C | VAL | A | 190 | 70.233 | 88.072 | 6.886 | 1.00 | 29.41 |
| 2503 | O | VAL | A | 190 | 69.586 | 87.448 | 6.037 | 1.00 | 29.64 |
| 2504 | N | PRO | A | 191 | 71.501 | 88.441 | 6.701 | 1.00 | 29.70 |
| 2505 | CA | PRO | A | 191 | 72.217 | 88.146 | 5.458 | 1.00 | 29.74 |
| 2507 | CB | PRO | A | 191 | 73.565 | 88.851 | 5.643 | 1.00 | 29.72 |
| 2510 | CG | PRO | A | 191 | 73.389 | 89.766 | 6.777 | 1.00 | 30.18 |
| 2513 | CD | PRO | A | 191 | 72.357 | 89.168 | 7.653 | 1.00 | 30.09 |
| 2516 | C | PRO | A | 191 | 72.448 | 86.659 | 5.266 | 1.00 | 29.95 |
| 2517 | O | PRO | A | 191 | 72.317 | 85.896 | 6.224 | 1.00 | 29.23 |
| 2518 | N | LEU | A | 192 | 72.843 | 86.279 | 4.059 | 1.00 | 30.11 |
| 2520 | CA | LEU | A | 192 | 73.010 | 84.873 | 3.690 | 1.00 | 30.66 |
| 2522 | CB | LEU | A | 192 | 73.595 | 84.765 | 2.281 | 1.00 | 30.90 |
| 2525 | CG | LEU | A | 192 | 73.604 | 83.417 | 1.548 | 1.00 | 32.07 |
| 2527 | CD1 | LEU | A | 192 | 74.931 | 82.695 | 1.750 | 1.00 | 34.56 |
| 2531 | CD2 | LEU | A | 192 | 72.438 | 82.535 | 1.942 | 1.00 | 31.83 |
| 2535 | C | LEU | A | 192 | 73.875 | 84.071 | 4.670 | 1.00 | 30.74 |
| 2536 | O | LEU | A | 192 | 73.472 | 82.997 | 5.093 | 1.00 | 30.04 |
| 2537 | N | ASP | A | 193 | 75.058 | 84.584 | 5.009 | 1.00 | 30.98 |
| 2539 | CA | ASP | A | 193 | 75.951 | 83.903 | 5.945 | 1.00 | 31.77 |
| 2541 | CB | ASP | A | 193 | 77.278 | 84.667 | 6.143 | 1.00 | 32.58 |
| 2544 | CG | ASP | A | 193 | 77.097 | 86.128 | 6.641 | 1.00 | 34.74 |
| 2545 | OD1 | ASP | A | 193 | 75.963 | 86.630 | 6.812 | 1.00 | 37.70 |
| 2546 | OD2 | ASP | A | 193 | 78.079 | 86.866 | 6.881 | 1.00 | 39.45 |
| 2547 | C | ASP | A | 193 | 75.295 | 83.578 | 7.301 | 1.00 | 31.43 |
| 2548 | O | ASP | A | 193 | 75.516 | 82.494 | 7.847 | 1.00 | 31.36 |
| 2549 | N | ALA | A | 194 | 74.493 | 84.505 | 7.823 | 1.00 | 30.71 |
| 2551 | CA | ALA | A | 194 | 73.781 | 84.297 | 9.082 | 1.00 | 30.32 |
| 2553 | CB | ALA | A | 194 | 73.271 | 85.624 | 9.641 | 1.00 | 30.46 |
| 2557 | C | ALA | A | 194 | 72.627 | 83.331 | 8.870 | 1.00 | 29.80 |
| 2558 | O | ALA | A | 194 | 72.328 | 82.505 | 9.731 | 1.00 | 28.47 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 2559 | N | LEU | A | 195 | 71.990 | 83.427 | 7.708 | 1.00 | 29.23 |
| 2561 | CA | LEU | A | 195 | 70.902 | 82.529 | 7.358 | 1.00 | 29.70 |
| 2563 | CB | LEU | A | 195 | 70.360 | 82.867 | 5.971 | 1.00 | 30.15 |
| 2566 | CG | LEU | A | 195 | 68.870 | 83.128 | 5.772 | 1.00 | 31.79 |
| 2568 | CD1 | LEU | A | 195 | 68.545 | 82.912 | 4.280 | 1.00 | 32.57 |
| 2572 | CD2 | LEU | A | 195 | 67.958 | 82.296 | 6.672 | 1.00 | 32.39 |
| 2576 | C | LEU | A | 195 | 71.397 | 81.077 | 7.356 | 1.00 | 29.25 |
| 2577 | O | LEU | A | 195 | 70.766 | 80.182 | 7.923 | 1.00 | 27.68 |
| 2578 | N | GLU | A | 196 | 72.539 | 80.867 | 6.712 | 1.00 | 28.91 |
| 2580 | CA | GLU | A | 196 | 73.138 | 79.547 | 6.604 | 1.00 | 28.82 |
| 2582 | CB | GLU | A | 196 | 74.362 | 79.609 | 5.697 | 1.00 | 29.44 |
| 2585 | CG | GLU | A | 196 | 74.926 | 78.249 | 5.322 | 1.00 | 31.65 |
| 2588 | CD | GLU | A | 196 | 76.119 | 78.345 | 4.382 | 1.00 | 35.05 |
| 2589 | OE1 | GLU | A | 196 | 76.048 | 79.127 | 3.405 | 1.00 | 36.65 |
| 2590 | OE2 | GLU | A | 196 | 77.126 | 77.631 | 4.625 | 1.00 | 37.41 |
| 2591 | C | GLU | A | 196 | 73.524 | 78.996 | 7.972 | 1.00 | 28.22 |
| 2592 | O | GLU | A | 196 | 73.406 | 77.807 | 8.220 | 1.00 | 27.03 |
| 2593 | N | ARG | A | 197 | 74.001 | 79.866 | 8.856 | 1.00 | 27.79 |
| 2595 | CA | ARG | A | 197 | 74.342 | 79.454 | 10.210 | 1.00 | 27.69 |
| 2597 | CB | ARG | A | 197 | 75.021 | 80.585 | 10.988 | 1.00 | 28.29 |
| 2600 | CG | ARG | A | 197 | 76.429 | 80.908 | 10.483 | 1.00 | 32.30 |
| 2603 | CD | ARG | A | 197 | 77.323 | 81.682 | 11.474 | 1.00 | 35.96 |
| 2606 | NE | ARG | A | 197 | 78.509 | 80.902 | 11.831 | 1.00 | 39.49 |
| 2608 | CZ | ARG | A | 197 | 79.520 | 80.619 | 11.005 | 1.00 | 42.00 |
| 2609 | NH1 | ARG | A | 197 | 79.524 | 81.054 | 9.748 | 1.00 | 43.12 |
| 2612 | NH2 | ARG | A | 197 | 80.539 | 79.889 | 11.440 | 1.00 | 42.49 |
| 2615 | C | ARG | A | 197 | 73.100 | 78.970 | 10.948 | 1.00 | 26.20 |
| 2616 | O | ARG | A | 197 | 73.153 | 77.952 | 11.634 | 1.00 | 25.47 |
| 2617 | N | ILE | A | 198 | 71.985 | 79.681 | 10.787 | 1.00 | 25.12 |
| 2619 | CA | ILE | A | 198 | 70.719 | 79.254 | 11.387 | 1.00 | 24.45 |
| 2621 | CB | ILE | A | 198 | 69.546 | 80.183 | 11.009 | 1.00 | 24.28 |
| 2623 | CG1 | ILE | A | 198 | 69.717 | 81.579 | 11.619 | 1.00 | 25.03 |
| 2626 | CD1 | ILE | A | 198 | 68.851 | 82.624 | 10.981 | 1.00 | 25.02 |
| 2630 | CG2 | ILE | A | 198 | 68.222 | 79.577 | 11.474 | 1.00 | 24.54 |
| 2634 | C | ILE | A | 198 | 70.385 | 77.842 | 10.906 | 1.00 | 24.27 |
| 2635 | O | ILE | A | 198 | 70.205 | 76.928 | 11.699 | 1.00 | 23.05 |
| 2636 | N | HIS | A | 199 | 70.289 | 77.701 | 9.590 | 1.00 | 23.44 |
| 2638 | CA | HIS | A | 199 | 69.789 | 76.477 | 8.976 | 1.00 | 23.31 |
| 2640 | CB | HIS | A | 199 | 69.573 | 76.731 | 7.485 | 1.00 | 23.43 |
| 2643 | CG | HIS | A | 199 | 68.349 | 77.547 | 7.209 | 1.00 | 24.48 |
| 2644 | ND1 | HIS | A | 199 | 67.494 | 77.964 | 8.208 | 1.00 | 25.73 |
| 2646 | CE1 | HIS | A | 199 | 66.480 | 78.623 | 7.675 | 1.00 | 26.42 |
| 2648 | NE2 | HIS | A | 199 | 66.659 | 78.669 | 6.367 | 1.00 | 25.37 |
| 2650 | CD2 | HIS | A | 199 | 67.817 | 77.999 | 6.052 | 1.00 | 25.77 |
| 2652 | C | HIS | A | 199 | 70.678 | 75.264 | 9.230 | 1.00 | 22.37 |
| 2653 | O | HIS | A | 199 | 70.179 | 74.181 | 9.534 | 1.00 | 22.47 |
| 2654 | N | ARG | A | 200 | 71.986 | 75.445 | 9.128 | 1.00 | 21.53 |
| 2656 | CA | ARG | A | 200 | 72.919 | 74.362 | 9.391 | 1.00 | 21.47 |
| 2658 | CB | ARG | A | 200 | 74.358 | 74.778 | 9.120 | 1.00 | 20.83 |
| 2661 | CG | ARG | A | 200 | 74.700 | 74.835 | 7.656 | 1.00 | 21.22 |
| 2664 | CD | ARG | A | 200 | 76.180 | 74.847 | 7.423 | 1.00 | 22.88 |
| 2667 | NE | ARG | A | 200 | 76.501 | 75.077 | 6.022 | 1.00 | 24.27 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 2669 | CZ | ARG | A | 200 | 76.459 | 74.147 | 5.092 | 1.00 | 25.12 |
| 2670 | NH1 | ARG | A | 200 | 76.120 | 72.904 | 5.398 | 1.00 | 25.42 |
| 2673 | NH2 | ARG | A | 200 | 76.784 | 74.455 | 3.840 | 1.00 | 28.83 |
| 2676 | C | ARG | A | 200 | 72.780 | 73.872 | 10.829 | 1.00 | 21.18 |
| 2677 | O | ARG | A | 200 | 72.861 | 72.681 | 11.071 | 1.00 | 20.79 |
| 2678 | N | HIS | A | 201 | 72.583 | 74.777 | 11.784 | 1.00 | 21.00 |
| 2680 | CA | HIS | A | 201 | 72.436 | 74.337 | 13.171 | 1.00 | 21.63 |
| 2682 | CB | HIS | A | 201 | 72.773 | 75.458 | 14.158 | 1.00 | 21.62 |
| 2685 | CG | HIS | A | 201 | 74.232 | 75.787 | 14.215 | 1.00 | 24.46 |
| 2686 | ND1 | HIS | A | 201 | 74.944 | 75.833 | 15.394 | 1.00 | 28.06 |
| 2688 | CE1 | HIS | A | 201 | 76.201 | 76.148 | 15.134 | 1.00 | 28.87 |
| 2690 | NE2 | HIS | A | 201 | 76.330 | 76.304 | 13.831 | 1.00 | 29.50 |
| 2692 | CD2 | HIS | A | 201 | 75.113 | 76.086 | 13.233 | 1.00 | 27.40 |
| 2694 | C | HIS | A | 201 | 71.050 | 73.751 | 13.451 | 1.00 | 21.00 |
| 2695 | O | HIS | A | 201 | 70.948 | 72.646 | 13.985 | 1.00 | 20.86 |
| 2696 | N | LYS | A | 202 | 69.985 | 74.462 | 13.087 | 1.00 | 20.63 |
| 2698 | CA | LYS | A | 202 | 68.642 | 74.022 | 13.489 | 1.00 | 20.10 |
| 2700 | CB | LYS | A | 202 | 67.590 | 75.123 | 13.367 | 1.00 | 19.88 |
| 2703 | CG | LYS | A | 202 | 66.987 | 75.363 | 11.997 | 1.00 | 19.59 |
| 2706 | CD | LYS | A | 202 | 65.944 | 76.473 | 12.065 | 1.00 | 19.02 |
| 2709 | CE | LYS | A | 202 | 65.416 | 76.847 | 10.672 | 1.00 | 18.63 |
| 2712 | NZ | LYS | A | 202 | 64.064 | 77.494 | 10.673 | 1.00 | 19.09 |
| 2716 | C | LYS | A | 202 | 68.215 | 72.756 | 12.758 | 1.00 | 20.00 |
| 2717 | O | LYS | A | 202 | 67.491 | 71.960 | 13.307 | 1.00 | 20.23 |
| 2718 | N | THR | A | 203 | 68.705 | 72.557 | 11.539 | 1.00 | 19.63 |
| 2720 | CA | THR | A | 203 | 68.278 | 71.433 | 10.726 | 1.00 | 19.13 |
| 2722 | CB | THR | A | 203 | 67.408 | 71.938 | 9.580 | 1.00 | 19.35 |
| 2724 | OG1 | THR | A | 203 | 66.166 | 72.400 | 10.127 | 1.00 | 18.33 |
| 2726 | CG2 | THR | A | 203 | 67.021 | 70.812 | 8.618 | 1.00 | 18.67 |
| 2730 | C | THR | A | 203 | 69.413 | 70.554 | 10.226 | 1.00 | 19.03 |
| 2731 | O | THR | A | 203 | 69.275 | 69.332 | 10.223 | 1.00 | 18.17 |
| 2732 | N | GLY | A | 204 | 70.522 | 71.167 | 9.812 | 1.00 | 19.30 |
| 2734 | CA | GLY | A | 204 | 71.667 | 70.421 | 9.316 | 1.00 | 19.16 |
| 2737 | C | GLY | A | 204 | 72.260 | 69.466 | 10.329 | 1.00 | 19.28 |
| 2738 | O | GLY | A | 204 | 72.580 | 68.330 | 9.987 | 1.00 | 19.12 |
| 2739 | N | ALA | A | 205 | 72.371 | 69.910 | 11.576 | 1.00 | 19.18 |
| 2741 | CA | ALA | A | 205 | 73.129 | 69.182 | 12.585 | 1.00 | 19.36 |
| 2743 | CB | ALA | A | 205 | 73.245 | 70.005 | 13.861 | 1.00 | 19.70 |
| 2747 | C | ALA | A | 205 | 72.505 | 67.816 | 12.897 | 1.00 | 19.34 |
| 2748 | O | ALA | A | 205 | 73.224 | 66.830 | 13.057 | 1.00 | 19.28 |
| 2749 | N | LEU | A | 206 | 71.177 | 67.768 | 12.994 | 1.00 | 19.51 |
| 2751 | CA | LEU | A | 206 | 70.476 | 66.522 | 13.302 | 1.00 | 19.63 |
| 2753 | CB | LEU | A | 206 | 69.016 | 66.775 | 13.700 | 1.00 | 19.77 |
| 2756 | CG | LEU | A | 206 | 68.261 | 65.516 | 14.183 | 1.00 | 20.34 |
| 2758 | CD1 | LEU | A | 206 | 68.918 | 64.931 | 15.431 | 1.00 | 20.63 |
| 2762 | CD2 | LEU | A | 206 | 66.799 | 65.855 | 14.449 | 1.00 | 20.55 |
| 2766 | C | LEU | A | 206 | 70.514 | 65.563 | 12.125 | 1.00 | 19.55 |
| 2767 | O | LEU | A | 206 | 70.590 | 64.336 | 12.312 | 1.00 | 19.72 |
| 2768 | N | ILE | A | 207 | 70.462 | 66.114 | 10.919 | 1.00 | 19.19 |
| 2770 | CA | ILE | A | 207 | 70.556 | 65.299 | 9.706 | 1.00 | 19.51 |
| 2772 | CB | ILE | A | 207 | 70.178 | 66.143 | 8.471 | 1.00 | 19.64 |
| 2774 | CG1 | ILE | A | 207 | 68.659 | 66.197 | 8.372 | 1.00 | 20.21 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 2777 | CD1 | ILE | A | 207 | 68.149 | 67.249 | 7.449 | 1.00 | 21.65 |
| 2781 | CG2 | ILE | A | 207 | 70.782 | 65.578 | 7.169 | 1.00 | 20.92 |
| 2785 | C | ILE | A | 207 | 71.941 | 64.661 | 9.604 | 1.00 | 19.17 |
| 2786 | O | ILE | A | 207 | 72.066 | 63.504 | 9.227 | 1.00 | 18.77 |
| 2787 | N | ARG | A | 208 | 72.970 | 65.420 | 9.963 | 1.00 | 19.39 |
| 2789 | CA | ARG | A | 208 | 74.323 | 64.891 | 10.001 | 1.00 | 19.72 |
| 2791 | CB | ARG | A | 208 | 75.343 | 66.008 | 10.148 | 1.00 | 20.03 |
| 2794 | CG | ARG | A | 208 | 76.774 | 65.526 | 10.119 | 1.00 | 21.06 |
| 2797 | CD | ARG | A | 208 | 77.777 | 66.638 | 10.165 | 1.00 | 20.98 |
| 2800 | NE | ARG | A | 208 | 77.824 | 67.265 | 11.473 | 1.00 | 23.53 |
| 2802 | CZ | ARG | A | 208 | 78.617 | 68.294 | 11.789 | 1.00 | 25.30 |
| 2803 | NH1 | ARG | A | 208 | 78.580 | 68.800 | 13.012 | 1.00 | 23.66 |
| 2806 | NH2 | ARG | A | 208 | 79.445 | 68.815 | 10.891 | 1.00 | 26.69 |
| 2809 | C | ARG | A | 208 | 74.453 | 63.843 | 11.113 | 1.00 | 19.73 |
| 2810 | O | ARG | A | 208 | 75.153 | 62.859 | 10.935 | 1.00 | 19.84 |
| 2811 | N | ALA | A | 209 | 73.741 | 64.027 | 12.226 | 1.00 | 19.24 |
| 2813 | CA | ALA | A | 209 | 73.713 | 63.009 | 13.276 | 1.00 | 18.65 |
| 2815 | CB | ALA | A | 209 | 73.001 | 63.513 | 14.517 | 1.00 | 19.04 |
| 2819 | C | ALA | A | 209 | 73.097 | 61.696 | 12.824 | 1.00 | 18.20 |
| 2820 | O | ALA | A | 209 | 73.582 | 60.644 | 13.210 | 1.00 | 18.83 |
| 2821 | N | ALA | A | 210 | 72.025 | 61.740 | 12.043 | 1.00 | 18.01 |
| 2823 | CA | ALA | A | 210 | 71.441 | 60.524 | 11.485 | 1.00 | 18.08 |
| 2825 | CB | ALA | A | 210 | 70.268 | 60.868 | 10.588 | 1.00 | 18.17 |
| 2829 | C | ALA | A | 210 | 72.481 | 59.738 | 10.700 | 1.00 | 18.04 |
| 2830 | O | ALA | A | 210 | 72.645 | 58.522 | 10.879 | 1.00 | 17.73 |
| 2831 | N | VAL | A | 211 | 73.170 | 60.430 | 9.809 | 1.00 | 17.87 |
| 2833 | CA | VAL | A | 211 | 74.174 | 59.786 | 8.990 | 1.00 | 18.48 |
| 2835 | CB | VAL | A | 211 | 74.659 | 60.714 | 7.874 | 1.00 | 18.22 |
| 2837 | CG1 | VAL | A | 211 | 75.791 | 60.079 | 7.109 | 1.00 | 18.92 |
| 2841 | CG2 | VAL | A | 211 | 73.476 | 61.057 | 6.930 | 1.00 | 17.58 |
| 2845 | C | VAL | A | 211 | 75.314 | 59.238 | 9.852 | 1.00 | 18.69 |
| 2846 | O | VAL | A | 211 | 75.716 | 58.086 | 9.677 | 1.00 | 20.23 |
| 2847 | N | ARG | A | 212 | 75.783 | 60.032 | 10.808 | 1.00 | 18.74 |
| 2849 | CA | ARG | A | 212 | 76.862 | 59.629 | 11.702 | 1.00 | 18.96 |
| 2851 | CB | ARG | A | 212 | 77.274 | 60.778 | 12.615 | 1.00 | 18.76 |
| 2854 | CG | ARG | A | 212 | 78.157 | 61.792 | 11.948 | 1.00 | 19.71 |
| 2857 | CD | ARG | A | 212 | 78.477 | 63.008 | 12.803 | 1.00 | 19.66 |
| 2860 | NE | ARG | A | 212 | 79.481 | 63.857 | 12.167 | 1.00 | 21.03 |
| 2862 | CZ | ARG | A | 212 | 80.008 | 64.936 | 12.737 | 1.00 | 22.60 |
| 2863 | NH1 | ARG | A | 212 | 79.659 | 65.289 | 13.965 | 1.00 | 22.08 |
| 2866 | NH2 | ARG | A | 212 | 80.903 | 65.660 | 12.079 | 1.00 | 21.63 |
| 2869 | C | ARG | A | 212 | 76.481 | 58.427 | 12.549 | 1.00 | 19.18 |
| 2870 | O | ARG | A | 212 | 77.283 | 57.530 | 12.757 | 1.00 | 18.61 |
| 2871 | N | LEU | A | 213 | 75.244 | 58.394 | 13.014 | 1.00 | 19.73 |
| 2873 | CA | LEU | A | 213 | 74.790 | 57.288 | 13.850 | 1.00 | 20.29 |
| 2875 | CB | LEU | A | 213 | 73.426 | 57.600 | 14.481 | 1.00 | 20.21 |
| 2878 | CG | LEU | A | 213 | 73.432 | 58.067 | 15.944 | 1.00 | 21.69 |
| 2880 | CD1 | LEU | A | 213 | 74.453 | 59.147 | 16.210 | 1.00 | 22.70 |
| 2884 | CD2 | LEU | A | 213 | 72.044 | 58.554 | 16.298 | 1.00 | 23.52 |
| 2888 | C | LEU | A | 213 | 74.715 | 56.013 | 13.013 | 1.00 | 20.31 |
| 2889 | O | LEU | A | 213 | 75.049 | 54.941 | 13.486 | 1.00 | 19.90 |
| 2890 | N | GLY | A | 214 | 74.273 | 56.131 | 11.772 | 1.00 | 20.46 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 2892 | CA | GLY | A | 214 | 74.297 | 55.000 | 10.861 | 1.00 | 21.15 |
| 2895 | C | GLY | A | 214 | 75.703 | 54.457 | 10.656 | 1.00 | 21.20 |
| 2896 | O | GLY | A | 214 | 75.933 | 53.240 | 10.737 | 1.00 | 22.15 |
| 2897 | N | ALA | A | 215 | 76.643 | 55.362 | 10.419 | 1.00 | 21.27 |
| 2899 | CA | ALA | A | 215 | 78.046 | 55.006 | 10.215 | 1.00 | 22.05 |
| 2901 | CB | ALA | A | 215 | 78.813 | 56.193 | 9.733 | 1.00 | 21.96 |
| 2905 | C | ALA | A | 215 | 78.700 | 54.419 | 11.480 | 1.00 | 22.41 |
| 2906 | O | ALA | A | 215 | 79.383 | 53.398 | 11.411 | 1.00 | 22.53 |
| 2907 | N | LEU | A | 216 | 78.471 | 55.041 | 12.635 | 1.00 | 22.29 |
| 2909 | CA | LEU | A | 216 | 79.090 | 54.580 | 13.877 | 1.00 | 22.51 |
| 2911 | CB | LEU | A | 216 | 78.775 | 55.522 | 15.039 | 1.00 | 22.37 |
| 2914 | CG | LEU | A | 216 | 79.513 | 56.853 | 14.977 | 1.00 | 22.40 |
| 2916 | CD1 | LEU | A | 216 | 78.845 | 57.900 | 15.863 | 1.00 | 22.42 |
| 2920 | CD2 | LEU | A | 216 | 81.004 | 56.689 | 15.372 | 1.00 | 22.32 |
| 2924 | C | LEU | A | 216 | 78.642 | 53.168 | 14.213 | 1.00 | 23.22 |
| 2925 | O | LEU | A | 216 | 79.383 | 52.408 | 14.830 | 1.00 | 23.30 |
| 2926 | N | SER | A | 217 | 77.430 | 52.809 | 13.786 | 1.00 | 24.01 |
| 2928 | CA | SER | A | 217 | 76.914 | 51.469 | 13.999 | 1.00 | 24.10 |
| 2930 | CB | SER | A | 217 | 75.478 | 51.347 | 13.496 | 1.00 | 24.10 |
| 2933 | OG | SER | A | 217 | 75.459 | 51.162 | 12.104 | 1.00 | 25.59 |
| 2935 | C | SER | A | 217 | 77.764 | 50.397 | 13.335 | 1.00 | 24.24 |
| 2936 | O | SER | A | 217 | 77.746 | 49.254 | 13.778 | 1.00 | 23.60 |
| 2937 | N | ALA | A | 218 | 78.464 | 50.782 | 12.269 | 1.00 | 24.79 |
| 2939 | CA | ALA | A | 218 | 79.332 | 49.906 | 11.496 | 1.00 | 25.88 |
| 2941 | CB | ALA | A | 218 | 79.361 | 50.376 | 10.050 | 1.00 | 26.06 |
| 2945 | C | ALA | A | 218 | 80.762 | 49.837 | 12.044 | 1.00 | 26.25 |
| 2946 | O | ALA | A | 218 | 81.602 | 49.130 | 11.490 | 1.00 | 27.04 |
| 2947 | N | GLY | A | 219 | 81.051 | 50.586 | 13.100 | 1.00 | 26.38 |
| 2949 | CA | GLY | A | 219 | 82.373 | 50.574 | 13.692 | 1.00 | 27.08 |
| 2952 | C | GLY | A | 219 | 83.427 | 51.209 | 12.809 | 1.00 | 27.54 |
| 2953 | O | GLY | A | 219 | 83.193 | 52.242 | 12.199 | 1.00 | 27.58 |
| 2954 | N | ASP | A | 220 | 84.584 | 50.570 | 12.718 | 1.00 | 28.92 |
| 2956 | CA | ASP | A | 220 | 85.758 | 51.188 | 12.105 | 1.00 | 29.67 |
| 2958 | CB | ASP | A | 220 | 86.993 | 50.294 | 12.281 | 1.00 | 30.31 |
| 2961 | CG | ASP | A | 220 | 87.596 | 50.413 | 13.666 | 1.00 | 33.03 |
| 2962 | OD1 | ASP | A | 220 | 88.445 | 49.568 | 14.020 | 1.00 | 37.45 |
| 2963 | OD2 | ASP | A | 220 | 87.285 | 51.318 | 14.478 | 1.00 | 35.85 |
| 2964 | C | ASP | A | 220 | 85.530 | 51.523 | 10.650 | 1.00 | 29.40 |
| 2965 | O | ASP | A | 220 | 85.907 | 52.596 | 10.203 | 1.00 | 29.23 |
| 2966 | N | LYS | A | 221 | 84.879 | 50.625 | 9.921 | 1.00 | 29.50 |
| 2968 | CA | LYS | A | 221 | 84.593 | 50.862 | 8.505 | 1.00 | 29.92 |
| 2970 | CB | LYS | A | 221 | 84.019 | 49.610 | 7.839 | 1.00 | 30.45 |
| 2973 | CG | LYS | A | 221 | 85.103 | 48.766 | 7.182 | 1.00 | 33.43 |
| 2976 | CD | LYS | A | 221 | 84.685 | 47.310 | 6.964 | 1.00 | 36.17 |
| 2979 | CE | LYS | A | 221 | 85.888 | 46.439 | 6.568 | 1.00 | 37.55 |
| 2982 | NZ | LYS | A | 221 | 85.967 | 45.213 | 7.416 | 1.00 | 39.13 |
| 2986 | C | LYS | A | 221 | 83.672 | 52.076 | 8.312 | 1.00 | 29.02 |
| 2987 | O | LYS | A | 221 | 83.851 | 52.860 | 7.384 | 1.00 | 27.84 |
| 2988 | N | GLY | A | 222 | 82.696 | 52.241 | 9.198 | 1.00 | 28.66 |
| 2990 | CA | GLY | A | 222 | 81.855 | 53.429 | 9.162 | 1.00 | 28.17 |
| 2993 | C | GLY | A | 222 | 82.647 | 54.692 | 9.471 | 1.00 | 27.77 |
| 2994 | O | GLY | A | 222 | 82.503 | 55.719 | 8.812 | 1.00 | 27.08 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 2995 | N | ARG | A | 223 | 83.498 | 54.609 | 10.482 | 1.00 | 27.98 |
| 2997 | CA | ARG | A | 223 | 84.306 | 55.751 | 10.900 | 1.00 | 28.29 |
| 2999 | CB | ARG | A | 223 | 85.165 | 55.391 | 12.106 | 1.00 | 28.55 |
| 3002 | CG | ARG | A | 223 | 84.449 | 55.520 | 13.428 | 1.00 | 28.34 |
| 3005 | CD | ARG | A | 223 | 85.328 | 55.173 | 14.580 | 1.00 | 29.33 |
| 3008 | NE | ARG | A | 223 | 84.577 | 55.110 | 15.826 | 1.00 | 29.90 |
| 3010 | CZ | ARG | A | 223 | 84.375 | 56.148 | 16.637 | 1.00 | 29.01 |
| 3011 | NH1 | ARG | A | 223 | 84.836 | 57.359 | 16.334 | 1.00 | 29.10 |
| 3014 | NH2 | ARG | A | 223 | 83.671 | 55.980 | 17.743 | 1.00 | 28.00 |
| 3017 | C | ARG | A | 223 | 85.201 | 56.266 | 9.783 | 1.00 | 28.80 |
| 3018 | O | ARG | A | 223 | 85.367 | 57.476 | 9.645 | 1.00 | 28.97 |
| 3019 | N | ARG | A | 224 | 85.752 | 55.354 | 8.978 | 1.00 | 29.00 |
| 3021 | CA | ARG | A | 224 | 86.622 | 55.726 | 7.853 | 1.00 | 29.76 |
| 3023 | CB | ARG | A | 224 | 87.268 | 54.483 | 7.223 | 1.00 | 30.54 |
| 3026 | CG | ARG | A | 224 | 88.351 | 53.812 | 8.069 | 1.00 | 33.89 |
| 3029 | CD | ARG | A | 224 | 88.273 | 52.280 | 8.115 | 1.00 | 38.26 |
| 3032 | NE | ARG | A | 224 | 88.914 | 51.617 | 6.975 | 1.00 | 41.13 |
| 3034 | CZ | ARG | A | 224 | 88.318 | 51.290 | 5.817 | 1.00 | 44.61 |
| 3035 | NH1 | ARG | A | 224 | 89.023 | 50.681 | 4.862 | 1.00 | 46.06 |
| 3038 | NH2 | ARG | A | 224 | 87.037 | 51.564 | 5.587 | 1.00 | 45.97 |
| 3041 | C | ARG | A | 224 | 85.866 | 56.481 | 6.765 | 1.00 | 29.10 |
| 3042 | O | ARG | A | 224 | 86.460 | 57.283 | 6.034 | 1.00 | 29.09 |
| 3043 | N | ALA | A | 225 | 84.565 | 56.209 | 6.646 | 1.00 | 27.99 |
| 3045 | CA | ALA | A | 225 | 83.720 | 56.894 | 5.669 | 1.00 | 27.60 |
| 3047 | CB | ALA | A | 225 | 82.532 | 56.030 | 5.313 | 1.00 | 27.48 |
| 3051 | C | ALA | A | 225 | 83.234 | 58.253 | 6.142 | 1.00 | 27.24 |
| 3052 | O | ALA | A | 225 | 82.710 | 59.018 | 5.344 | 1.00 | 26.75 |
| 3053 | N | LEU | A | 226 | 83.394 | 58.543 | 7.433 | 1.00 | 27.30 |
| 3055 | CA | LEU | A | 226 | 82.807 | 59.736 | 8.036 | 1.00 | 27.51 |
| 3057 | CB | LEU | A | 226 | 83.061 | 59.804 | 9.546 | 1.00 | 27.81 |
| 3060 | CG | LEU | A | 226 | 82.127 | 58.960 | 10.416 | 1.00 | 29.69 |
| 3062 | CD1 | LEU | A | 226 | 82.573 | 59.004 | 11.889 | 1.00 | 30.50 |
| 3066 | CD2 | LEU | A | 226 | 80.677 | 59.411 | 10.271 | 1.00 | 30.60 |
| 3070 | C | LEU | A | 226 | 83.226 | 61.045 | 7.400 | 1.00 | 26.87 |
| 3071 | O | LEU | A | 226 | 82.380 | 61.901 | 7.232 | 1.00 | 27.16 |
| 3072 | N | PRO | A | 227 | 84.502 | 61.248 | 7.067 | 1.00 | 26.59 |
| 3073 | CA | PRO | A | 227 | 84.879 | 62.502 | 6.399 | 1.00 | 26.30 |
| 3075 | CB | PRO | A | 227 | 86.349 | 62.269 | 6.006 | 1.00 | 26.54 |
| 3078 | CG | PRO | A | 227 | 86.853 | 61.366 | 7.081 | 1.00 | 27.08 |
| 3081 | CD | PRO | A | 227 | 85.685 | 60.415 | 7.352 | 1.00 | 26.58 |
| 3084 | C | PRO | A | 227 | 83.996 | 62.758 | 5.195 | 1.00 | 25.66 |
| 3085 | O | PRO | A | 227 | 83.479 | 63.859 | 5.044 | 1.00 | 26.22 |
| 3086 | N | VAL | A | 228 | 83.770 | 61.735 | 4.381 | 1.00 | 24.71 |
| 3088 | CA | VAL | A | 228 | 82.965 | 61.910 | 3.181 | 1.00 | 24.34 |
| 3090 | CB | VAL | A | 228 | 83.272 | 60.835 | 2.139 | 1.00 | 24.09 |
| 3092 | CG1 | VAL | A | 228 | 82.302 | 60.927 | 0.999 | 1.00 | 23.94 |
| 3096 | CG2 | VAL | A | 228 | 84.718 | 60.988 | 1.655 | 1.00 | 25.44 |
| 3100 | C | VAL | A | 228 | 81.465 | 61.955 | 3.470 | 1.00 | 23.78 |
| 3101 | O | VAL | A | 228 | 80.754 | 62.771 | 2.885 | 1.00 | 23.40 |
| 3102 | N | LEU | A | 229 | 80.978 | 61.096 | 4.362 | 1.00 | 23.25 |
| 3104 | CA | LEU | A | 229 | 79.552 | 61.118 | 4.707 | 1.00 | 22.90 |
| 3106 | CB | LEU | A | 229 | 79.179 | 59.955 | 5.627 | 1.00 | 23.13 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 3109 | CG | LEU | A | 229 | 79.130 | 58.583 | 4.947 | 1.00 | 22.78 |
| 3111 | CD1 | LEU | A | 229 | 79.022 | 57.462 | 5.987 | 1.00 | 23.57 |
| 3115 | CD2 | LEU | A | 229 | 77.991 | 58.484 | 3.975 | 1.00 | 23.72 |
| 3119 | C | LEU | A | 229 | 79.159 | 62.441 | 5.346 | 1.00 | 23.02 |
| 3120 | O | LEU | A | 229 | 78.023 | 62.903 | 5.182 | 1.00 | 22.74 |
| 3121 | N | ASP | A | 230 | 80.081 | 63.036 | 6.093 | 1.00 | 23.24 |
| 3123 | CA | ASP | A | 230 | 79.838 | 64.328 | 6.722 | 1.00 | 23.61 |
| 3125 | CB | ASP | A | 230 | 81.028 | 64.753 | 7.588 | 1.00 | 23.94 |
| 3128 | CG | ASP | A | 230 | 81.009 | 64.118 | 8.974 | 1.00 | 25.27 |
| 3129 | OD1 | ASP | A | 230 | 79.961 | 63.561 | 9.379 | 1.00 | 25.31 |
| 3130 | OD2 | ASP | A | 230 | 81.989 | 64.158 | 9.749 | 1.00 | 27.02 |
| 3131 | C | ASP | A | 230 | 79.568 | 65.385 | 5.654 | 1.00 | 23.60 |
| 3132 | O | ASP | A | 230 | 78.630 | 66.175 | 5.772 | 1.00 | 22.89 |
| 3133 | N | LYS | A | 231 | 80.373 | 65.377 | 4.599 | 1.00 | 23.58 |
| 3135 | CA | LYS | A | 231 | 80.234 | 66.391 | 3.557 | 1.00 | 24.32 |
| 3137 | CB | LYS | A | 231 | 81.439 | 66.381 | 2.594 | 1.00 | 24.94 |
| 3140 | CG | LYS | A | 231 | 82.825 | 66.478 | 3.298 | 1.00 | 27.64 |
| 3143 | CD | LYS | A | 231 | 83.113 | 67.828 | 4.009 | 1.00 | 31.84 |
| 3146 | CE | LYS | A | 231 | 83.516 | 67.719 | 5.546 | 1.00 | 32.28 |
| 3149 | NZ | LYS | A | 231 | 84.063 | 66.374 | 6.064 | 1.00 | 30.63 |
| 3153 | C | LYS | A | 231 | 78.901 | 66.207 | 2.842 | 1.00 | 23.43 |
| 3154 | O | LYS | A | 231 | 78.205 | 67.177 | 2.548 | 1.00 | 23.79 |
| 3155 | N | TYR | A | 232 | 78.521 | 64.955 | 2.612 | 1.00 | 22.64 |
| 3157 | CA | TYR | A | 232 | 77.214 | 64.632 | 2.063 | 1.00 | 21.59 |
| 3159 | CB | TYR | A | 232 | 77.075 | 63.114 | 1.881 | 1.00 | 21.93 |
| 3162 | CG | TYR | A | 232 | 75.645 | 62.633 | 1.753 | 1.00 | 20.62 |
| 3163 | CD1 | TYR | A | 232 | 75.021 | 62.606 | 0.523 | 1.00 | 21.37 |
| 3165 | CE1 | TYR | A | 232 | 73.736 | 62.160 | 0.386 | 1.00 | 20.90 |
| 3167 | CZ | TYR | A | 232 | 73.030 | 61.727 | 1.487 | 1.00 | 20.66 |
| 3168 | OH | TYR | A | 232 | 71.737 | 61.289 | 1.311 | 1.00 | 21.67 |
| 3170 | CE2 | TYR | A | 232 | 73.617 | 61.727 | 2.730 | 1.00 | 21.12 |
| 3172 | CD2 | TYR | A | 232 | 74.933 | 62.174 | 2.862 | 1.00 | 20.69 |
| 3174 | C | TYR | A | 232 | 76.098 | 65.121 | 2.979 | 1.00 | 21.19 |
| 3175 | O | TYR | A | 232 | 75.156 | 65.754 | 2.523 | 1.00 | 21.30 |
| 3176 | N | ALA | A | 233 | 76.208 | 64.804 | 4.261 | 1.00 | 20.68 |
| 3178 | CA | ALA | A | 233 | 75.173 | 65.126 | 5.240 | 1.00 | 20.41 |
| 3180 | CB | ALA | A | 233 | 75.503 | 64.513 | 6.581 | 1.00 | 20.07 |
| 3184 | C | ALA | A | 233 | 75.007 | 66.627 | 5.390 | 1.00 | 20.36 |
| 3185 | O | ALA | A | 233 | 73.893 | 67.123 | 5.485 | 1.00 | 19.95 |
| 3186 | N | GLU | A | 234 | 76.132 | 67.326 | 5.407 | 1.00 | 20.85 |
| 3188 | CA | GLU | A | 234 | 76.160 | 68.786 | 5.503 | 1.00 | 21.65 |
| 3190 | CB | GLU | A | 234 | 77.601 | 69.285 | 5.581 | 1.00 | 21.59 |
| 3193 | CG | GLU | A | 234 | 78.225 | 69.020 | 6.940 | 1.00 | 23.51 |
| 3196 | CD | GLU | A | 234 | 79.737 | 68.868 | 6.911 | 1.00 | 25.72 |
| 3197 | OE1 | GLU | A | 234 | 80.292 | 68.333 | 7.899 | 1.00 | 25.16 |
| 3198 | OE2 | GLU | A | 234 | 80.367 | 69.272 | 5.910 | 1.00 | 28.53 |
| 3199 | C | GLU | A | 234 | 75.411 | 69.428 | 4.340 | 1.00 | 21.53 |
| 3200 | O | GLU | A | 234 | 74.644 | 70.370 | 4.532 | 1.00 | 22.09 |
| 3201 | N | SER | A | 235 | 75.600 | 68.899 | 3.141 | 1.00 | 21.49 |
| 3203 | CA | SER | A | 235 | 74.922 | 69.459 | 1.985 | 1.00 | 21.57 |
| 3205 | CB | SER | A | 235 | 75.598 | 69.036 | 0.695 | 1.00 | 21.17 |
| 3208 | OG | SER | A | 235 | 76.870 | 69.647 | 0.589 | 1.00 | 22.38 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 3210 | C | SER | A | 235 | 73.432 | 69.119 | 1.967 | 1.00 | 21.32 |
| 3211 | O | SER | A | 235 | 72.629 | 69.993 | 1.719 | 1.00 | 20.51 |
| 3212 | N | ILE | A | 236 | 73.044 | 67.871 | 2.238 | 1.00 | 21.52 |
| 3214 | CA | ILE | A | 236 | 71.610 | 67.562 | 2.236 | 1.00 | 21.70 |
| 3216 | CB | ILE | A | 236 | 71.318 | 66.049 | 2.154 | 1.00 | 21.58 |
| 3218 | CG1 | ILE | A | 236 | 71.881 | 65.279 | 3.347 | 1.00 | 22.85 |
| 3221 | CD1 | ILE | A | 236 | 71.069 | 64.038 | 3.669 | 1.00 | 22.81 |
| 3225 | CG2 | ILE | A | 236 | 71.815 | 65.486 | 0.849 | 1.00 | 21.97 |
| 3229 | C | ILE | A | 236 | 70.874 | 68.190 | 3.421 | 1.00 | 21.12 |
| 3230 | O | ILE | A | 236 | 69.684 | 68.467 | 3.337 | 1.00 | 21.31 |
| 3231 | N | GLY | A | 237 | 71.583 | 68.412 | 4.520 | 1.00 | 21.08 |
| 3233 | CA | GLY | A | 237 | 70.983 | 68.977 | 5.714 | 1.00 | 21.32 |
| 3236 | C | GLY | A | 237 | 70.607 | 70.441 | 5.534 | 1.00 | 21.14 |
| 3237 | O | GLY | A | 237 | 69.514 | 70.877 | 5.917 | 1.00 | 21.86 |
| 3238 | N | LEU | A | 238 | 71.513 | 71.205 | 4.939 | 1.00 | 21.35 |
| 3240 | CA | LEU | A | 238 | 71.214 | 72.583 | 4.595 | 1.00 | 21.18 |
| 3242 | CB | LEU | A | 238 | 72.467 | 73.318 | 4.127 | 1.00 | 21.49 |
| 3245 | CG | LEU | A | 238 | 72.250 | 74.769 | 3.712 | 1.00 | 21.63 |
| 3247 | CD1 | LEU | A | 238 | 71.601 | 75.564 | 4.829 | 1.00 | 22.56 |
| 3251 | CD2 | LEU | A | 238 | 73.571 | 75.361 | 3.320 | 1.00 | 23.37 |
| 3255 | C | LEU | A | 238 | 70.134 | 72.604 | 3.521 | 1.00 | 20.95 |
| 3256 | O | LEU | A | 238 | 69.171 | 73.324 | 3.659 | 1.00 | 20.57 |
| 3257 | N | ALA | A | 239 | 70.270 | 71.766 | 2.488 | 1.00 | 20.80 |
| 3259 | CA | ALA | A | 239 | 69.271 | 71.677 | 1.424 | 1.00 | 20.94 |
| 3261 | CB | ALA | A | 239 | 69.674 | 70.639 | 0.373 | 1.00 | 21.23 |
| 3265 | C | ALA | A | 239 | 67.885 | 71.350 | 1.966 | 1.00 | 20.81 |
| 3266 | O | ALA | A | 239 | 66.878 | 71.812 | 1.442 | 1.00 | 20.67 |
| 3267 | N | PHE | A | 240 | 67.840 | 70.554 | 3.029 | 1.00 | 20.67 |
| 3269 | CA | PHE | A | 240 | 66.568 | 70.166 | 3.634 | 1.00 | 20.70 |
| 3271 | CB | PHE | A | 240 | 66.798 | 69.201 | 4.785 | 1.00 | 20.78 |
| 3274 | CG | PHE | A | 240 | 65.600 | 68.375 | 5.131 | 1.00 | 22.14 |
| 3275 | CD1 | PHE | A | 240 | 65.546 | 67.041 | 4.768 | 1.00 | 23.74 |
| 3277 | CE1 | PHE | A | 240 | 64.455 | 66.267 | 5.103 | 1.00 | 25.17 |
| 3279 | CZ | PHE | A | 240 | 63.407 | 66.817 | 5.797 | 1.00 | 23.85 |
| 3281 | CE2 | PHE | A | 240 | 63.462 | 68.143 | 6.173 | 1.00 | 23.26 |
| 3283 | CD2 | PHE | A | 240 | 64.551 | 68.907 | 5.851 | 1.00 | 21.11 |
| 3285 | C | PHE | A | 240 | 65.812 | 71.378 | 4.147 | 1.00 | 20.30 |
| 3286 | O | PHE | A | 240 | 64.590 | 71.496 | 3.939 | 1.00 | 19.63 |
| 3287 | N | GLN | A | 241 | 66.523 | 72.269 | 4.835 | 1.00 | 20.63 |
| 3289 | CA | GLN | A | 241 | 65.874 | 73.456 | 5.381 | 1.00 | 21.12 |
| 3291 | CB | GLN | A | 241 | 66.699 | 74.091 | 6.503 | 1.00 | 21.39 |
| 3294 | CG | GLN | A | 241 | 65.944 | 75.205 | 7.276 | 1.00 | 21.45 |
| 3297 | CD | GLN | A | 241 | 64.668 | 74.715 | 7.926 | 1.00 | 23.00 |
| 3298 | OE1 | GLN | A | 241 | 64.650 | 73.654 | 8.548 | 1.00 | 23.23 |
| 3299 | NE2 | GLN | A | 241 | 63.595 | 75.490 | 7.795 | 1.00 | 20.99 |
| 3302 | C | GLN | A | 241 | 65.546 | 74.494 | 4.300 | 1.00 | 21.77 |
| 3303 | O | GLN | A | 241 | 64.511 | 75.148 | 4.375 | 1.00 | 22.39 |
| 3304 | N | VAL | A | 242 | 66.402 | 74.641 | 3.299 | 1.00 | 22.51 |
| 3306 | CA | VAL | A | 242 | 66.066 | 75.543 | 2.184 | 1.00 | 22.92 |
| 3308 | CB | VAL | A | 242 | 67.260 | 75.840 | 1.212 | 1.00 | 23.27 |
| 3310 | CG1 | VAL | A | 242 | 68.054 | 74.664 | 0.922 | 1.00 | 26.25 |
| 3314 | CG2 | VAL | A | 242 | 66.794 | 76.486 | -0.102 | 1.00 | 23.71 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 3318 | C | VAL | A | 242 | 64.794 | 75.075 | 1.478 | 1.00 | 22.84 |
| 3319 | O | VAL | A | 242 | 63.936 | 75.893 | 1.150 | 1.00 | 22.34 |
| 3320 | N | GLN | A | 243 | 64.635 | 73.761 | 1.307 | 1.00 | 23.02 |
| 3322 | CA | GLN | A | 243 | 63.413 | 73.222 | 0.738 | 1.00 | 23.04 |
| 3324 | CB | GLN | A | 243 | 63.538 | 71.727 | 0.418 | 1.00 | 23.87 |
| 3327 | CG | GLN | A | 243 | 62.276 | 71.128 | -0.198 | 1.00 | 25.59 |
| 3330 | CD | GLN | A | 243 | 62.058 | 71.593 | -1.623 | 1.00 | 29.42 |
| 3331 | OE1 | GLN | A | 243 | 62.818 | 72.426 | -2.133 | 1.00 | 30.57 |
| 3332 | NE2 | GLN | A | 243 | 61.025 | 71.053 | -2.275 | 1.00 | 28.29 |
| 3335 | C | GLN | A | 243 | 62.241 | 73.441 | 1.671 | 1.00 | 22.23 |
| 3336 | O | GLN | A | 243 | 61.140 | 73.709 | 1.213 | 1.00 | 22.37 |
| 3337 | N | ASP | A | 244 | 62.467 | 73.315 | 2.977 | 1.00 | 21.60 |
| 3339 | CA | ASP | A | 244 | 61.409 | 73.564 | 3.954 | 1.00 | 21.14 |
| 3341 | CB | ASP | A | 244 | 61.898 | 73.263 | 5.372 | 1.00 | 20.81 |
| 3344 | CG | ASP | A | 244 | 60.808 | 73.400 | 6.393 | 1.00 | 20.15 |
| 3345 | OD1 | ASP | A | 244 | 59.877 | 72.588 | 6.376 | 1.00 | 22.40 |
| 3346 | OD2 | ASP | A | 244 | 60.774 | 74.310 | 7.250 | 1.00 | 23.26 |
| 3347 | C | ASP | A | 244 | 60.904 | 75.018 | 3.848 | 1.00 | 21.37 |
| 3348 | O | ASP | A | 244 | 59.701 | 75.260 | 3.866 | 1.00 | 21.86 |
| 3349 | N | ASP | A | 245 | 61.820 | 75.966 | 3.694 | 1.00 | 21.89 |
| 3351 | CA | ASP | A | 245 | 61.446 | 77.379 | 3.534 | 1.00 | 22.75 |
| 3353 | CB | ASP | A | 245 | 62.674 | 78.275 | 3.478 | 1.00 | 22.66 |
| 3356 | CG | ASP | A | 245 | 63.436 | 78.375 | 4.789 | 1.00 | 23.92 |
| 3357 | OD1 | ASP | A | 245 | 62.965 | 77.899 | 5.859 | 1.00 | 26.27 |
| 3358 | OD2 | ASP | A | 245 | 64.542 | 78.966 | 4.821 | 1.00 | 23.49 |
| 3359 | C | ASP | A | 245 | 60.679 | 77.596 | 2.219 | 1.00 | 23.14 |
| 3360 | O | ASP | A | 245 | 59.719 | 78.357 | 2.158 | 1.00 | 23.09 |
| 3361 | N | ILE | A | 246 | 61.129 | 76.934 | 1.162 | 1.00 | 24.22 |
| 3363 | CA | ILE | A | 246 | 60.507 | 77.067 | -0.150 | 1.00 | 24.50 |
| 3365 | CB | ILE | A | 246 | 61.358 | 76.356 | -1.230 | 1.00 | 24.79 |
| 3367 | CG1 | ILE | A | 246 | 62.593 | 77.200 | -1.545 | 1.00 | 25.00 |
| 3370 | CD1 | ILE | A | 246 | 63.697 | 76.444 | -2.246 | 1.00 | 25.62 |
| 3374 | CG2 | ILE | A | 246 | 60.548 | 76.118 | -2.518 | 1.00 | 24.83 |
| 3378 | C | ILE | A | 246 | 59.094 | 76.529 | -0.095 | 1.00 | 24.74 |
| 3379 | O | ILE | A | 246 | 58.168 | 77.162 | -0.598 | 1.00 | 24.41 |
| 3380 | N | LEU | A | 247 | 58.920 | 75.380 | 0.561 | 1.00 | 24.90 |
| 3382 | CA | LEU | A | 247 | 57.608 | 74.763 | 0.702 | 1.00 | 25.47 |
| 3384 | CB | LEU | A | 247 | 57.721 | 73.376 | 1.346 | 1.00 | 25.41 |
| 3387 | CG | LEU | A | 247 | 58.364 | 72.296 | 0.469 | 1.00 | 26.20 |
| 3389 | CD1 | LEU | A | 247 | 58.592 | 71.012 | 1.275 | 1.00 | 26.19 |
| 3393 | CD2 | LEU | A | 247 | 57.523 | 72.032 | -0.762 | 1.00 | 26.28 |
| 3397 | C | LEU | A | 247 | 56.677 | 75.637 | 1.517 | 1.00 | 25.82 |
| 3398 | O | LEU | A | 247 | 55.463 | 75.646 | 1.296 | 1.00 | 26.02 |
| 3399 | N | ASP | A | 248 | 57.238 | 76.375 | 2.461 | 1.00 | 26.06 |
| 3401 | CA | ASP | A | 248 | 56.422 | 77.233 | 3.298 | 1.00 | 27.02 |
| 3403 | CB | ASP | A | 248 | 57.239 | 77.832 | 4.426 | 1.00 | 26.69 |
| 3406 | CG | ASP | A | 248 | 56.390 | 78.176 | 5.607 | 1.00 | 28.82 |
| 3407 | OD1 | ASP | A | 248 | 55.886 | 79.319 | 5.636 | 1.00 | 29.75 |
| 3408 | OD2 | ASP | A | 248 | 56.148 | 77.365 | 6.534 | 1.00 | 31.49 |
| 3409 | C | ASP | A | 248 | 55.765 | 78.333 | 2.458 | 1.00 | 27.65 |
| 3410 | O | ASP | A | 248 | 54.622 | 78.689 | 2.698 | 1.00 | 28.08 |
| 3411 | N | VAL | A | 249 | 56.481 | 78.823 | 1.454 | 1.00 | 28.57 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 3413 | CA | VAL | A | 249 | 55.949 | 79.838 | 0.542 | 1.00 | 29.59 |
| 3415 | CB | VAL | A | 249 | 57.091 | 80.577 | -0.188 | 1.00 | 29.49 |
| 3417 | CG1 | VAL | A | 249 | 56.537 | 81.656 | -1.140 | 1.00 | 29.98 |
| 3421 | CG2 | VAL | A | 249 | 58.062 | 81.200 | 0.825 | 1.00 | 29.51 |
| 3425 | C | VAL | A | 249 | 54.951 | 79.248 | -0.477 | 1.00 | 30.63 |
| 3426 | O | VAL | A | 249 | 53.791 | 79.669 | -0.525 | 1.00 | 30.78 |
| 3427 | N | VAL | A | 250 | 55.388 | 78.253 | -1.250 | 1.00 | 31.44 |
| 3429 | CA | VAL | A | 250 | 54.642 | 77.785 | -2.427 | 1.00 | 32.17 |
| 3431 | CB | VAL | A | 250 | 55.605 | 77.525 | -3.617 | 1.00 | 32.40 |
| 3433 | CG1 | VAL | A | 250 | 56.588 | 78.680 | -3.768 | 1.00 | 32.66 |
| 3437 | CG2 | VAL | A | 250 | 56.349 | 76.185 | -3.462 | 1.00 | 32.82 |
| 3441 | C | VAL | A | 250 | 53.766 | 76.543 | -2.233 | 1.00 | 32.47 |
| 3442 | O | VAL | A | 250 | 52.963 | 76.204 | -3.110 | 1.00 | 32.70 |
| 3443 | N | GLY | A | 251 | 53.915 | 75.854 | -1.105 | 1.00 | 32.77 |
| 3445 | CA | GLY | A | 251 | 53.200 | 74.611 | -0.879 | 1.00 | 33.14 |
| 3448 | C | GLY | A | 251 | 51.784 | 74.871 | -0.407 | 1.00 | 33.82 |
| 3449 | O | GLY | A | 251 | 51.515 | 75.920 | 0.162 | 1.00 | 34.10 |
| 3450 | N | ASP | A | 252 | 50.887 | 73.920 | -0.656 | 1.00 | 34.38 |
| 3452 | CA | ASP | A | 252 | 49.489 | 73.995 | -0.211 | 1.00 | 34.75 |
| 3454 | CB | ASP | A | 252 | 48.602 | 73.159 | -1.151 | 1.00 | 35.30 |
| 3457 | CG | ASP | A | 252 | 47.185 | 73.699 | -1.272 | 1.00 | 38.65 |
| 3458 | OD1 | ASP | A | 252 | 46.738 | 73.925 | -2.425 | 1.00 | 42.04 |
| 3459 | OD2 | ASP | A | 252 | 46.433 | 73.914 | -0.284 | 1.00 | 42.91 |
| 3460 | C | ASP | A | 252 | 49.431 | 73.410 | 1.198 | 1.00 | 33.97 |
| 3461 | O | ASP | A | 252 | 50.088 | 72.411 | 1.456 | 1.00 | 33.79 |
| 3462 | N | THR | A | 253 | 48.643 | 74.009 | 2.089 | 1.00 | 33.08 |
| 3464 | CA | THR | A | 253 | 48.489 | 73.517 | 3.465 | 1.00 | 32.87 |
| 3466 | CB | THR | A | 253 | 47.476 | 74.394 | 4.249 | 1.00 | 32.46 |
| 3468 | OG1 | THR | A | 253 | 48.002 | 75.710 | 4.420 | 1.00 | 32.70 |
| 3470 | CG2 | THR | A | 253 | 47.288 | 73.901 | 5.684 | 1.00 | 32.42 |
| 3474 | C | THR | A | 253 | 48.061 | 72.041 | 3.542 | 1.00 | 32.67 |
| 3475 | O | THR | A | 253 | 48.561 | 71.297 | 4.377 | 1.00 | 32.65 |
| 3476 | N | ALA | A | 254 | 47.141 | 71.617 | 2.677 | 1.00 | 32.34 |
| 3478 | CA | ALA | A | 254 | 46.651 | 70.240 | 2.709 | 1.00 | 32.14 |
| 3480 | CB | ALA | A | 254 | 45.388 | 70.095 | 1.857 | 1.00 | 32.51 |
| 3484 | C | ALA | A | 254 | 47.724 | 69.228 | 2.271 | 1.00 | 31.60 |
| 3485 | O | ALA | A | 254 | 47.692 | 68.073 | 2.678 | 1.00 | 31.38 |
| 3486 | N | THR | A | 255 | 48.668 | 69.666 | 1.447 | 1.00 | 31.12 |
| 3488 | CA | THR | A | 255 | 49.785 | 68.815 | 1.025 | 1.00 | 31.09 |
| 3490 | CB | THR | A | 255 | 50.269 | 69.251 | -0.371 | 1.00 | 31.32 |
| 3492 | OG1 | THR | A | 255 | 49.192 | 69.112 | -1.313 | 1.00 | 33.79 |
| 3494 | CG2 | THR | A | 255 | 51.348 | 68.308 | -0.917 | 1.00 | 31.41 |
| 3498 | C | THR | A | 255 | 50.943 | 68.825 | 2.045 | 1.00 | 30.23 |
| 3499 | O | THR | A | 255 | 51.483 | 67.768 | 2.391 | 1.00 | 30.03 |
| 3500 | N | LEU | A | 256 | 51.312 | 70.017 | 2.520 | 1.00 | 29.30 |
| 3502 | CA | LEU | A | 256 | 52.358 | 70.175 | 3.539 | 1.00 | 28.64 |
| 3504 | CB | LEU | A | 256 | 52.668 | 71.653 | 3.766 | 1.00 | 28.31 |
| 3507 | CG | LEU | A | 256 | 53.253 | 72.412 | 2.577 | 1.00 | 29.19 |
| 3509 | CD1 | LEU | A | 256 | 53.329 | 73.903 | 2.883 | 1.00 | 29.07 |
| 3513 | CD2 | LEU | A | 256 | 54.620 | 71.880 | 2.197 | 1.00 | 29.56 |
| 3517 | C | LEU | A | 256 | 52.007 | 69.554 | 4.880 | 1.00 | 27.73 |
| 3518 | O | LEU | A | 256 | 52.877 | 69.038 | 5.578 | 1.00 | 27.92 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 3519 | N | GLY | A | 257 | 50.732 | 69.613 | 5.240 | 1.00 | 26.76 |
| 3521 | CA | GLY | A | 257 | 50.277 | 69.195 | 6.546 | 1.00 | 26.19 |
| 3524 | C | GLY | A | 257 | 50.485 | 70.266 | 7.601 | 1.00 | 25.80 |
| 3525 | O | GLY | A | 257 | 50.150 | 70.053 | 8.757 | 1.00 | 24.95 |
| 3526 | N | LYS | A | 258 | 51.071 | 71.388 | 7.197 | 1.00 | 25.86 |
| 3528 | CA | LYS | A | 258 | 51.273 | 72.556 | 8.052 | 1.00 | 26.53 |
| 3530 | CB | LYS | A | 258 | 52.701 | 72.588 | 8.628 | 1.00 | 25.80 |
| 3533 | CG | LYS | A | 258 | 53.804 | 72.498 | 7.579 | 1.00 | 25.64 |
| 3536 | CD | LYS | A | 258 | 55.183 | 72.231 | 8.200 | 1.00 | 23.61 |
| 3539 | CE | LYS | A | 258 | 56.297 | 72.507 | 7.205 | 1.00 | 22.86 |
| 3542 | NZ | LYS | A | 258 | 57.604 | 71.866 | 7.602 | 1.00 | 21.94 |
| 3546 | C | LYS | A | 258 | 50.992 | 73.813 | 7.223 | 1.00 | 27.55 |
| 3547 | O | LYS | A | 258 | 51.046 | 73.781 | 5.982 | 1.00 | 28.12 |
| 3548 | N | ARG | A | 259 | 50.721 | 74.918 | 7.905 | 1.00 | 28.61 |
| 3550 | CA | ARG | A | 259 | 50.217 | 76.128 | 7.249 | 1.00 | 29.63 |
| 3552 | CB | ARG | A | 259 | 49.658 | 77.096 | 8.287 | 1.00 | 30.10 |
| 3555 | CG | ARG | A | 259 | 48.370 | 76.612 | 8.875 | 1.00 | 32.12 |
| 3558 | CD | ARG | A | 259 | 47.441 | 77.693 | 9.362 | 1.00 | 35.28 |
| 3561 | NE | ARG | A | 259 | 46.380 | 77.104 | 10.175 | 1.00 | 38.07 |
| 3563 | CZ | ARG | A | 259 | 45.308 | 76.476 | 9.688 | 1.00 | 40.08 |
| 3564 | NH1 | ARG | A | 259 | 45.095 | 76.378 | 8.376 | 1.00 | 39.60 |
| 3567 | NH2 | ARG | A | 259 | 44.419 | 75.962 | 10.533 | 1.00 | 40.97 |
| 3570 | C | ARG | A | 259 | 51.223 | 76.852 | 6.360 | 1.00 | 29.71 |
| 3571 | O | ARG | A | 259 | 52.306 | 77.274 | 6.806 | 1.00 | 29.38 |
| 3572 | N | GLN | A | 260 | 50.847 | 76.966 | 5.084 | 1.00 | 30.10 |
| 3574 | CA | GLN | A | 260 | 51.544 | 77.794 | 4.108 | 1.00 | 29.94 |
| 3576 | CB | GLN | A | 260 | 50.816 | 77.731 | 2.754 | 1.00 | 30.17 |
| 3579 | CG | GLN | A | 260 | 51.436 | 78.643 | 1.649 | 1.00 | 31.83 |
| 3582 | CD | GLN | A | 260 | 50.618 | 78.716 | 0.357 | 1.00 | 34.25 |
| 3583 | OE1 | GLN | A | 260 | 51.157 | 79.057 | -0.705 | 1.00 | 35.57 |
| 3584 | NE2 | GLN | A | 260 | 49.333 | 78.396 | 0.439 | 1.00 | 35.68 |
| 3587 | C | GLN | A | 260 | 51.586 | 79.238 | 4.601 | 1.00 | 29.79 |
| 3588 | O | GLN | A | 260 | 50.625 | 79.733 | 5.193 | 1.00 | 29.82 |
| 3589 | N | GLY | A | 261 | 52.705 | 79.907 | 4.369 | 1.00 | 29.23 |
| 3591 | CA | GLY | A | 261 | 52.843 | 81.298 | 4.740 | 1.00 | 29.36 |
| 3594 | C | GLY | A | 261 | 53.063 | 81.513 | 6.230 | 1.00 | 29.17 |
| 3595 | O | GLY | A | 261 | 52.963 | 82.630 | 6.708 | 1.00 | 28.41 |
| 3596 | N | ALA | A | 262 | 53.372 | 80.453 | 6.971 | 1.00 | 29.32 |
| 3598 | CA | ALA | A | 262 | 53.670 | 80.594 | 8.395 | 1.00 | 29.31 |
| 3600 | CB | ALA | A | 262 | 53.865 | 79.216 | 9.032 | 1.00 | 29.54 |
| 3604 | C | ALA | A | 262 | 54.900 | 81.481 | 8.638 | 1.00 | 29.48 |
| 3605 | O | ALA | A | 262 | 54.915 | 82.276 | 9.569 | 1.00 | 30.09 |
| 3606 | N | ASP | A | 263 | 55.925 | 81.350 | 7.805 | 1.00 | 29.41 |
| 3608 | CA | ASP | A | 263 | 57.170 | 82.079 | 8.006 | 1.00 | 29.43 |
| 3610 | CB | ASP | A | 263 | 58.242 | 81.581 | 7.053 | 1.00 | 29.35 |
| 3613 | CG | ASP | A | 263 | 58.770 | 80.208 | 7.420 | 1.00 | 28.93 |
| 3614 | OD1 | ASP | A | 263 | 58.493 | 79.724 | 8.552 | 1.00 | 27.10 |
| 3615 | OD2 | ASP | A | 263 | 59.480 | 79.562 | 6.613 | 1.00 | 25.07 |
| 3616 | C | ASP | A | 263 | 56.992 | 83.576 | 7.772 | 1.00 | 30.15 |
| 3617 | O | ASP | A | 263 | 57.516 | 84.404 | 8.505 | 1.00 | 28.74 |
| 3618 | N | GLN | A | 264 | 56.258 | 83.887 | 6.717 | 1.00 | 31.27 |
| 3620 | CA | GLN | A | 264 | 56.003 | 85.254 | 6.311 | 1.00 | 32.11 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 3622 | CB | BGLN | A | 264 | 55.223 | 85.271 | 4.997 | 0.35 | 32.00 |
| 3623 | CB | AGLN | A | 264 | 55.313 | 85.259 | 4.930 | 0.65 | 32.18 |
| 3628 | CG | BGLN | A | 264 | 55.115 | 86.632 | 4.342 | 0.35 | 31.76 |
| 3629 | CG | AGLN | A | 264 | 56.317 | 84.920 | 3.801 | 0.65 | 32.43 |
| 3634 | CD | BGLN | A | 264 | 54.771 | 86.519 | 2.876 | 0.35 | 31.23 |
| 3635 | CD | AGLN | A | 264 | 55.724 | 84.264 | 2.547 | 0.65 | 32.97 |
| 3636 | OE1 | BGLN | A | 264 | 55.645 | 86.639 | 2.016 | 0.35 | 30.93 |
| 3637 | OE1 | AGLN | A | 264 | 54.977 | 83.279 | 2.618 | 0.65 | 32.08 |
| 3638 | NE2 | BGLN | A | 264 | 53.503 | 86.266 | 2.585 | 0.35 | 30.18 |
| 3639 | NE2 | AGLN | A | 264 | 56.103 | 84.792 | 1.389 | 0.65 | 33.37 |
| 3644 | C | GLN | A | 264 | 55.203 | 85.967 | 7.400 | 1.00 | 32.82 |
| 3645 | O | GLN | A | 264 | 55.460 | 87.123 | 7.720 | 1.00 | 33.46 |
| 3646 | N | GLN | A | 265 | 54.266 | 85.249 | 8.000 | 1.00 | 33.70 |
| 3648 | CA | GLN | A | 265 | 53.452 | 85.780 | 9.084 | 1.00 | 34.64 |
| 3650 | CB | GLN | A | 265 | 52.395 | 84.756 | 9.463 | 1.00 | 35.35 |
| 3653 | CG | GLN | A | 265 | 51.346 | 85.257 | 10.436 | 1.00 | 38.57 |
| 3656 | CD | GLN | A | 265 | 50.161 | 84.331 | 10.482 | 1.00 | 42.61 |
| 3657 | OE1 | GLN | A | 265 | 49.161 | 84.555 | 9.787 | 1.00 | 45.33 |
| 3658 | NE2 | GLN | A | 265 | 50.272 | 83.263 | 11.278 | 1.00 | 44.63 |
| 3661 | C | GLN | A | 265 | 54.281 | 86.173 | 10.320 | 1.00 | 34.20 |
| 3662 | O | GLN | A | 265 | 53.948 | 87.154 | 10.990 | 1.00 | 33.93 |
| 3663 | N | LEU | A | 266 | 55.347 | 85.419 | 10.613 | 1.00 | 33.21 |
| 3665 | CA | LEU | A | 266 | 56.247 | 85.737 | 11.734 | 1.00 | 32.74 |
| 3667 | CB | LEU | A | 266 | 56.676 | 84.463 | 12.474 | 1.00 | 32.73 |
| 3670 | CG | LEU | A | 266 | 55.629 | 83.549 | 13.112 | 1.00 | 34.09 |
| 3672 | CD1 | LEU | A | 266 | 56.300 | 82.734 | 14.206 | 1.00 | 35.07 |
| 3676 | CD2 | LEU | A | 266 | 54.412 | 84.295 | 13.676 | 1.00 | 35.20 |
| 3680 | C | LEU | A | 266 | 57.514 | 86.495 | 11.326 | 1.00 | 31.74 |
| 3681 | O | LEU | A | 266 | 58.348 | 86.790 | 12.172 | 1.00 | 31.90 |
| 3682 | N | GLY | A | 267 | 57.670 | 86.808 | 10.043 | 1.00 | 30.66 |
| 3684 | CA | GLY | A | 267 | 58.858 | 87.495 | 9.565 | 1.00 | 29.51 |
| 3687 | C | GLY | A | 267 | 60.157 | 86.732 | 9.759 | 1.00 | 28.74 |
| 3688 | O | GLY | A | 267 | 61.198 | 87.333 | 9.998 | 1.00 | 28.52 |
| 3689 | N | LYS | A | 268 | 60.099 | 85.405 | 9.649 | 1.00 | 27.62 |
| 3691 | CA | LYS | A | 268 | 61.296 | 84.575 | 9.707 | 1.00 | 26.77 |
| 3693 | CB | LYS | A | 268 | 60.934 | 83.092 | 9.572 | 1.00 | 26.29 |
| 3696 | CG | LYS | A | 268 | 60.021 | 82.536 | 10.642 | 1.00 | 25.90 |
| 3699 | CD | LYS | A | 268 | 60.797 | 82.141 | 11.884 | 1.00 | 26.17 |
| 3702 | CE | LYS | A | 268 | 59.882 | 81.593 | 12.965 | 1.00 | 26.68 |
| 3705 | NZ | LYS | A | 268 | 60.644 | 81.319 | 14.214 | 1.00 | 25.74 |
| 3709 | C | LYS | A | 268 | 62.280 | 84.943 | 8.595 | 1.00 | 26.39 |
| 3710 | O | LYS | A | 268 | 61.884 | 85.161 | 7.445 | 1.00 | 26.03 |
| 3711 | N | SER | A | 269 | 63.563 | 85.005 | 8.943 | 1.00 | 26.23 |
| 3713 | CA | SER | A | 269 | 64.629 | 85.019 | 7.944 | 1.00 | 26.10 |
| 3715 | CB | SER | A | 269 | 65.975 | 85.311 | 8.586 | 1.00 | 26.43 |
| 3718 | OG | SER | A | 269 | 65.979 | 86.581 | 9.207 | 1.00 | 26.96 |
| 3720 | C | SER | A | 269 | 64.666 | 83.652 | 7.247 | 1.00 | 26.21 |
| 3721 | O | SER | A | 269 | 64.899 | 82.629 | 7.898 | 1.00 | 25.19 |
| 3722 | N | THR | A | 270 | 64.388 | 83.642 | 5.942 | 1.00 | 25.65 |
| 3724 | CA | THR | A | 270 | 64.408 | 82.408 | 5.149 | 1.00 | 25.89 |
| 3726 | CB | THR | A | 270 | 62.975 | 81.922 | 4.812 | 1.00 | 26.14 |
| 3728 | OG1 | THR | A | 270 | 62.368 | 82.789 | 3.847 | 1.00 | 26.91 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 3730 | CG2 | THR | A | 270 | 62.046 | 81.992 | 6.033 | 1.00 | 26.45 |
| 3734 | C | THR | A | 270 | 65.189 | 82.591 | 3.856 | 1.00 | 25.77 |
| 3735 | O | THR | A | 270 | 65.538 | 83.722 | 3.472 | 1.00 | 25.52 |
| 3736 | N | TYR | A | 271 | 65.479 | 81.471 | 3.195 | 1.00 | 25.31 |
| 3738 | CA | TYR | A | 271 | 66.114 | 81.507 | 1.886 | 1.00 | 25.24 |
| 3740 | CB | TYR | A | 271 | 66.555 | 80.104 | 1.428 | 1.00 | 24.84 |
| 3743 | CG | TYR | A | 271 | 67.953 | 79.767 | 1.902 | 1.00 | 24.29 |
| 3744 | CD1 | TYR | A | 271 | 69.012 | 79.698 | 1.010 | 1.00 | 23.63 |
| 3746 | CE1 | TYR | A | 271 | 70.282 | 79.407 | 1.423 | 1.00 | 24.04 |
| 3748 | CZ | TYR | A | 271 | 70.545 | 79.200 | 2.759 | 1.00 | 24.29 |
| 3749 | OH | TYR | A | 271 | 71.827 | 78.928 | 3.168 | 1.00 | 24.41 |
| 3751 | CE2 | TYR | A | 271 | 69.521 | 79.276 | 3.685 | 1.00 | 24.92 |
| 3753 | CD2 | TYR | A | 271 | 68.225 | 79.566 | 3.250 | 1.00 | 23.77 |
| 3755 | C | TYR | A | 271 | 65.240 | 82.222 | 0.843 | 1.00 | 25.25 |
| 3756 | O | TYR | A | 271 | 65.717 | 83.149 | 0.211 | 1.00 | 25.83 |
| 3757 | N | PRO | A | 272 | 63.982 | 81.823 | 0.658 | 1.00 | 25.61 |
| 3758 | CA | PRO | A | 272 | 63.108 | 82.515 | -0.307 | 1.00 | 25.70 |
| 3760 | CB | PRO | A | 272 | 61.812 | 81.700 | -0.284 | 1.00 | 26.04 |
| 3763 | CG | PRO | A | 272 | 61.876 | 80.854 | 0.923 | 1.00 | 26.04 |
| 3766 | CD | PRO | A | 272 | 63.311 | 80.683 | 1.293 | 1.00 | 25.37 |
| 3769 | C | PRO | A | 272 | 62.825 | 83.980 | 0.027 | 1.00 | 25.95 |
| 3770 | O | PRO | A | 272 | 62.702 | 84.784 | -0.900 | 1.00 | 25.00 |
| 3771 | N | ALA | A | 273 | 62.738 | 84.326 | 1.311 | 1.00 | 26.04 |
| 3773 | CA | ALA | A | 273 | 62.503 | 85.719 | 1.697 | 1.00 | 26.33 |
| 3775 | CB | ALA | A | 273 | 62.193 | 85.853 | 3.166 | 1.00 | 26.37 |
| 3779 | C | ALA | A | 273 | 63.694 | 86.578 | 1.309 | 1.00 | 26.47 |
| 3780 | O | ALA | A | 273 | 63.512 | 87.637 | 0.734 | 1.00 | 26.90 |
| 3781 | N | LEU | A | 274 | 64.906 | 86.094 | 1.574 | 1.00 | 26.35 |
| 3783 | CA | LEU | A | 274 | 66.124 | 86.814 | 1.213 | 1.00 | 26.27 |
| 3785 | CB | LEU | A | 274 | 67.337 | 86.201 | 1.924 | 1.00 | 26.30 |
| 3788 | CG | LEU | A | 274 | 68.691 | 86.873 | 1.690 | 1.00 | 27.65 |
| 3790 | CD1 | LEU | A | 274 | 68.728 | 88.322 | 2.211 | 1.00 | 28.07 |
| 3794 | CD2 | LEU | A | 274 | 69.803 | 86.053 | 2.316 | 1.00 | 28.26 |
| 3798 | C | LEU | A | 274 | 66.386 | 86.828 | -0.294 | 1.00 | 26.01 |
| 3799 | O | LEU | A | 274 | 66.541 | 87.899 | -0.898 | 1.00 | 25.44 |
| 3800 | N | LEU | A | 275 | 66.439 | 85.633 | -0.881 | 1.00 | 25.58 |
| 3802 | CA | LEU | A | 275 | 66.963 | 85.430 | -2.234 | 1.00 | 25.43 |
| 3804 | CB | LEU | A | 275 | 67.755 | 84.113 | -2.298 | 1.00 | 25.44 |
| 3807 | CG | LEU | A | 275 | 68.906 | 83.896 | -1.320 | 1.00 | 26.67 |
| 3809 | CD1 | LEU | A | 275 | 69.520 | 82.486 | -1.510 | 1.00 | 25.96 |
| 3813 | CD2 | LEU | A | 275 | 69.960 | 84.976 | -1.479 | 1.00 | 27.24 |
| 3817 | C | LEU | A | 275 | 65.902 | 85.380 | -3.316 | 1.00 | 24.91 |
| 3818 | O | LEU | A | 275 | 66.226 | 85.454 | -4.490 | 1.00 | 24.92 |
| 3819 | N | GLY | A | 276 | 64.640 | 85.253 | -2.933 | 1.00 | 24.87 |
| 3821 | CA | GLY | A | 276 | 63.584 | 84.945 | -3.884 | 1.00 | 24.94 |
| 3824 | C | GLY | A | 276 | 63.529 | 83.446 | -4.151 | 1.00 | 25.33 |
| 3825 | O | GLY | A | 276 | 64.488 | 82.724 | -3.871 | 1.00 | 25.08 |
| 3826 | N | LEU | A | 277 | 62.415 | 82.985 | -4.699 | 1.00 | 25.79 |
| 3828 | CA | LEU | A | 277 | 62.170 | 81.567 | -4.899 | 1.00 | 26.67 |
| 3830 | CB | LEU | A | 277 | 60.732 | 81.320 | -5.383 | 1.00 | 27.35 |
| 3833 | CG | LEU | A | 277 | 59.602 | 81.477 | -4.365 | 1.00 | 28.42 |
| 3835 | CD1 | LEU | A | 277 | 58.252 | 81.403 | -5.068 | 1.00 | 29.93 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 3839 | CD2 | LEU | A | 277 | 59.687 | 80.413 | -3.279 | 1.00 | 28.63 |
| 3843 | C | LEU | A | 277 | 63.162 | 80.914 | -5.853 | 1.00 | 27.13 |
| 3844 | O | LEU | A | 277 | 63.593 | 79.796 | -5.591 | 1.00 | 27.11 |
| 3845 | N | GLU | A | 278 | 63.536 | 81.599 | -6.938 | 1.00 | 27.48 |
| 3847 | CA | GLU | A | 278 | 64.429 | 81.018 | -7.956 | 1.00 | 28.05 |
| 3849 | CB | GLU | A | 278 | 64.488 | 81.905 | -9.229 | 1.00 | 28.98 |
| 3852 | CG | GLU | A | 278 | 65.687 | 81.611 | -10.148 | 1.00 | 31.69 |
| 3855 | CD | GLU | A | 278 | 65.592 | 82.253 | -11.528 | 1.00 | 35.38 |
| 3856 | OE1 | GLU | A | 278 | 66.103 | 81.648 | -12.499 | 1.00 | 39.00 |
| 3857 | OE2 | GLU | A | 278 | 65.013 | 83.354 | -11.655 | 1.00 | 37.35 |
| 3858 | C | GLU | A | 278 | 65.850 | 80.739 | -7.455 | 1.00 | 27.43 |
| 3859 | O | GLU | A | 278 | 66.427 | 79.668 | -7.745 | 1.00 | 27.14 |
| 3860 | N | GLN | A | 279 | 66.432 | 81.697 | -6.743 | 1.00 | 26.16 |
| 3862 | CA | GLN | A | 279 | 67.799 | 81.563 | -6.250 | 1.00 | 26.17 |
| 3864 | CB | GLN | A | 279 | 68.364 | 82.909 | -5.793 | 1.00 | 26.14 |
| 3867 | CG | GLN | A | 279 | 68.642 | 83.881 | -6.920 | 1.00 | 29.26 |
| 3870 | CD | GLN | A | 279 | 69.025 | 85.266 | -6.418 | 1.00 | 32.23 |
| 3871 | OE1 | GLN | A | 279 | 69.828 | 85.405 | -5.485 | 1.00 | 34.54 |
| 3872 | NE2 | GLN | A | 279 | 68.464 | 86.295 | -7.046 | 1.00 | 34.59 |
| 3875 | C | GLN | A | 279 | 67.854 | 80.566 | -5.092 | 1.00 | 25.40 |
| 3876 | O | GLN | A | 279 | 68.856 | 79.905 | -4.900 | 1.00 | 25.15 |
| 3877 | N | ALA | A | 280 | 66.776 | 80.485 | -4.318 | 1.00 | 25.33 |
| 3879 | CA | ALA | A | 280 | 66.681 | 79.514 | -3.239 | 1.00 | 25.32 |
| 3881 | CB | ALA | A | 280 | 65.429 | 79.770 | -2.427 | 1.00 | 25.59 |
| 3885 | C | ALA | A | 280 | 66.665 | 78.097 | -3.837 | 1.00 | 25.68 |
| 3886 | O | ALA | A | 280 | 67.388 | 77.213 | -3.385 | 1.00 | 25.35 |
| 3887 | N | ARG | A | 281 | 65.860 | 77.913 | -4.878 | 1.00 | 25.78 |
| 3889 | CA | ARG | A | 281 | 65.753 | 76.631 | -5.564 | 1.00 | 26.49 |
| 3891 | CB | ARG | A | 281 | 64.725 | 76.697 | -6.683 | 1.00 | 26.59 |
| 3894 | CG | ARG | A | 281 | 63.311 | 76.604 | -6.197 | 1.00 | 27.19 |
| 3897 | CD | ARG | A | 281 | 62.284 | 76.791 | -7.294 | 1.00 | 29.91 |
| 3900 | NE | ARG | A | 281 | 60.926 | 76.575 | -6.799 | 1.00 | 31.85 |
| 3902 | CZ | ARG | A | 281 | 59.886 | 77.379 | -7.009 | 1.00 | 34.22 |
| 3903 | NH1 | ARG | A | 281 | 59.998 | 78.504 | -7.720 | 1.00 | 35.16 |
| 3906 | NH2 | ARG | A | 281 | 58.706 | 77.047 | -6.491 | 1.00 | 35.99 |
| 3909 | C | ARG | A | 281 | 67.091 | 76.201 | -6.109 | 1.00 | 26.94 |
| 3910 | O | ARG | A | 281 | 67.468 | 75.039 | -5.985 | 1.00 | 27.03 |
| 3911 | N | LYS | A | 282 | 67.816 | 77.155 | -6.679 | 1.00 | 27.58 |
| 3913 | CA | LYS | A | 282 | 69.145 | 76.929 | -7.218 | 1.00 | 28.35 |
| 3915 | CB | LYS | A | 282 | 69.641 | 78.193 | -7.934 | 1.00 | 29.25 |
| 3918 | CG | LYS | A | 282 | 71.101 | 78.163 | -8.408 | 1.00 | 31.10 |
| 3921 | CD | LYS | A | 282 | 71.288 | 77.283 | -9.637 | 1.00 | 34.04 |
| 3924 | CE | LYS | A | 282 | 72.514 | 77.689 | -10.473 | 1.00 | 35.05 |
| 3927 | NZ | LYS | A | 282 | 73.803 | 77.493 | -9.748 | 1.00 | 35.48 |
| 3931 | C | LYS | A | 282 | 70.130 | 76.552 | -6.132 | 1.00 | 28.37 |
| 3932 | O | LYS | A | 282 | 70.987 | 75.692 | -6.347 | 1.00 | 28.80 |
| 3933 | N | LYS | A | 283 | 70.054 | 77.222 | -4.986 | 1.00 | 28.08 |
| 3935 | CA | LYS | A | 283 | 70.938 | 76.890 | -3.873 | 1.00 | 27.92 |
| 3937 | CB | LYS | A | 283 | 70.723 | 77.824 | -2.675 | 1.00 | 28.22 |
| 3940 | CG | LYS | A | 283 | 71.163 | 79.279 | -2.921 | 1.00 | 30.08 |
| 3943 | CD | LYS | A | 283 | 72.546 | 79.581 | -2.376 | 1.00 | 31.98 |
| 3946 | CE | LYS | A | 283 | 72.871 | 81.085 | -2.414 | 1.00 | 32.86 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 3949 | NZ | LYS | A | 283 | 74.277 | 81.323 | -2.846 | 1.00 | 33.80 |
| 3953 | C | LYS | A | 283 | 70.680 | 75.438 | -3.453 | 1.00 | 27.24 |
| 3954 | O | LYS | A | 283 | 71.620 | 74.699 | -3.201 | 1.00 | 26.52 |
| 3955 | N | ALA | A | 284 | 69.411 | 75.041 | -3.393 | 1.00 | 26.71 |
| 3957 | CA | ALA | A | 284 | 69.053 | 73.682 | -2.960 | 1.00 | 26.99 |
| 3959 | CB | ALA | A | 284 | 67.544 | 73.546 | -2.823 | 1.00 | 26.84 |
| 3963 | C | ALA | A | 284 | 69.589 | 72.651 | -3.949 | 1.00 | 27.26 |
| 3964 | O | ALA | A | 284 | 70.141 | 71.636 | -3.566 | 1.00 | 26.69 |
| 3965 | N | ARG | A | 285 | 69.427 | 72.948 | -5.234 | 1.00 | 27.61 |
| 3967 | CA | ARG | A | 285 | 69.869 | 72.070 | -6.311 | 1.00 | 28.16 |
| 3969 | CB | ARG | A | 285 | 69.332 | 72.603 | -7.641 | 1.00 | 28.87 |
| 3972 | CG | ARG | A | 285 | 69.910 | 71.996 | -8.886 | 1.00 | 32.19 |
| 3975 | CD | ARG | A | 285 | 69.160 | 72.414 | -10.158 | 1.00 | 35.33 |
| 3978 | NE | ARG | A | 285 | 68.039 | 73.319 | -9.871 | 1.00 | 38.00 |
| 3980 | CZ | ARG | A | 285 | 68.005 | 74.632 | -10.133 | 1.00 | 38.95 |
| 3981 | NH1 | ARG | A | 285 | 69.027 | 75.256 | -10.711 | 1.00 | 40.27 |
| 3984 | NH2 | ARG | A | 285 | 66.924 | 75.329 | -9.815 | 1.00 | 38.71 |
| 3987 | C | ARG | A | 285 | 71.389 | 71.923 | -6.336 | 1.00 | 27.24 |
| 3988 | O | ARG | A | 285 | 71.885 | 70.819 | -6.512 | 1.00 | 27.02 |
| 3989 | N | ASP | A | 286 | 72.116 | 73.021 | -6.128 | 1.00 | 26.36 |
| 3991 | CA | ASP | A | 286 | 73.586 | 72.995 | -6.059 | 1.00 | 25.90 |
| 3993 | CB | ASP | A | 286 | 74.150 | 74.420 | -6.005 | 1.00 | 26.39 |
| 3996 | CG | ASP | A | 286 | 74.006 | 75.175 | -7.335 | 1.00 | 28.03 |
| 3997 | OD1 | ASP | A | 286 | 74.090 | 76.423 | -7.315 | 1.00 | 30.25 |
| 3998 | OD2 | ASP | A | 286 | 73.790 | 74.623 | -8.433 | 1.00 | 28.83 |
| 3999 | C | ASP | A | 286 | 74.086 | 72.217 | -4.828 | 1.00 | 25.37 |
| 4000 | O | ASP | A | 286 | 75.128 | 71.557 | -4.873 | 1.00 | 24.74 |
| 4001 | N | LEU | A | 287 | 73.346 | 72.307 | -3.727 | 1.00 | 24.45 |
| 4003 | CA | LEU | A | 287 | 73.688 | 71.553 | -2.529 | 1.00 | 24.47 |
| 4005 | CB | LEU | A | 287 | 72.825 | 71.999 | -1.335 | 1.00 | 24.55 |
| 4008 | CG | LEU | A | 287 | 73.246 | 73.324 | -0.700 | 1.00 | 23.94 |
| 4010 | CD1 | LEU | A | 287 | 72.129 | 73.904 | 0.129 | 1.00 | 23.80 |
| 4014 | CD2 | LEU | A | 287 | 74.506 | 73.133 | 0.150 | 1.00 | 23.78 |
| 4018 | C | LEU | A | 287 | 73.526 | 70.048 | -2.781 | 1.00 | 24.25 |
| 4019 | O | LEU | A | 287 | 74.364 | 69.262 | -2.353 | 1.00 | 23.54 |
| 4020 | N | ILE | A | 288 | 72.459 | 69.660 | -3.475 | 1.00 | 24.75 |
| 4022 | CA | ILE | A | 288 | 72.221 | 68.242 | -3.788 | 1.00 | 25.66 |
| 4024 | CB | ILE | A | 288 | 70.771 | 67.998 | -4.289 | 1.00 | 25.32 |
| 4026 | CG1 | ILE | A | 288 | 69.745 | 68.291 | -3.185 | 1.00 | 25.41 |
| 4029 | CD1 | ILE | A | 288 | 70.153 | 67.917 | -1.800 | 1.00 | 25.34 |
| 4033 | CG2 | ILE | A | 288 | 70.592 | 66.548 | -4.826 | 1.00 | 25.27 |
| 4037 | C | ILE | A | 288 | 73.241 | 67.719 | -4.788 | 1.00 | 26.42 |
| 4038 | O | ILE | A | 288 | 73.728 | 66.602 | -4.641 | 1.00 | 26.98 |
| 4039 | N | ASP | A | 289 | 73.571 | 68.511 | -5.802 | 1.00 | 27.38 |
| 4041 | CA | ASP | A | 289 | 74.607 | 68.111 | -6.753 | 1.00 | 28.16 |
| 4043 | CB | ASP | A | 289 | 74.799 | 69.165 | -7.851 | 1.00 | 28.99 |
| 4046 | CG | ASP | A | 289 | 73.578 | 69.319 | -8.758 | 1.00 | 31.72 |
| 4047 | OD1 | ASP | A | 289 | 73.510 | 70.341 | -9.477 | 1.00 | 36.96 |
| 4048 | OD2 | ASP | A | 289 | 72.644 | 68.493 | -8.830 | 1.00 | 35.17 |
| 4049 | C | ASP | A | 289 | 75.929 | 67.903 | -5.997 | 1.00 | 27.86 |
| 4050 | O | ASP | A | 289 | 76.696 | 67.003 | -6.319 | 1.00 | 27.48 |
| 4051 | N | ASP | A | 290 | 76.189 | 68.740 | -4.988 | 1.00 | 27.56 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 4053 | CA | ASP | A | 290 | 77.405 | 68.623 | -4.177 | 1.00 | 27.43 |
| 4055 | CB | ASP | A | 290 | 77.573 | 69.869 | -3.296 | 1.00 | 27.98 |
| 4058 | CG | ASP | A | 290 | 78.753 | 69.774 | -2.351 | 1.00 | 29.55 |
| 4059 | OD1 | ASP | A | 290 | 79.871 | 70.166 | -2.754 | 1.00 | 34.48 |
| 4060 | OD2 | ASP | A | 290 | 78.662 | 69.347 | -1.179 | 1.00 | 30.96 |
| 4061 | C | ASP | A | 290 | 77.344 | 67.351 | -3.320 | 1.00 | 26.91 |
| 4062 | O | ASP | A | 290 | 78.347 | 66.666 | -3.137 | 1.00 | 26.70 |
| 4063 | N | ALA | A | 291 | 76.154 | 67.039 | -2.817 | 1.00 | 26.35 |
| 4065 | CA | ALA | A | 291 | 75.935 | 65.830 | -2.041 | 1.00 | 26.26 |
| 4067 | CB | ALA | A | 291 | 74.514 | 65.811 | -1.452 | 1.00 | 26.18 |
| 4071 | C | ALA | A | 291 | 76.164 | 64.607 | -2.913 | 1.00 | 26.41 |
| 4072 | O | ALA | A | 291 | 76.774 | 63.648 | -2.469 | 1.00 | 26.46 |
| 4073 | N | ARG | A | 292 | 75.687 | 64.647 | -4.156 | 1.00 | 26.93 |
| 4075 | CA | ARG | A | 292 | 75.888 | 63.543 | -5.095 | 1.00 | 27.77 |
| 4077 | CB | ARG | A | 292 | 75.153 | 63.778 | -6.413 | 1.00 | 28.06 |
| 4080 | CG | ARG | A | 292 | 73.650 | 63.500 | -6.353 | 1.00 | 30.42 |
| 4083 | CD | ARG | A | 292 | 72.949 | 63.511 | -7.727 | 1.00 | 33.16 |
| 4086 | NE | ARG | A | 292 | 71.739 | 62.694 | -7.695 | 1.00 | 35.04 |
| 4088 | CZ | ARG | A | 292 | 71.709 | 61.365 | -7.828 | 1.00 | 37.56 |
| 4089 | NH1 | ARG | A | 292 | 72.820 | 60.653 | -8.041 | 1.00 | 37.77 |
| 4092 | NH2 | ARG | A | 292 | 70.544 | 60.731 | -7.757 | 1.00 | 37.95 |
| 4095 | C | ARG | A | 292 | 77.377 | 63.333 | -5.364 | 1.00 | 28.02 |
| 4096 | O | ARG | A | 292 | 77.837 | 62.202 | -5.438 | 1.00 | 27.64 |
| 4097 | N | GLN | A | 293 | 78.120 | 64.427 | -5.478 | 1.00 | 28.41 |
| 4099 | CA | GLN | A | 293 | 79.550 | 64.352 | -5.768 | 1.00 | 29.05 |
| 4101 | CB | GLN | A | 293 | 80.163 | 65.742 | -5.984 | 1.00 | 29.26 |
| 4104 | CG | GLN | A | 293 | 79.870 | 66.348 | -7.343 | 1.00 | 31.16 |
| 4107 | CD | GLN | A | 293 | 80.342 | 65.469 | -8.494 | 1.00 | 34.10 |
| 4108 | OE1 | GLN | A | 293 | 81.544 | 65.280 | -8.687 | 1.00 | 36.57 |
| 4109 | NE2 | GLN | A | 293 | 79.396 | 64.921 | -9.248 | 1.00 | 34.65 |
| 4112 | C | GLN | A | 293 | 80.260 | 63.638 | -4.645 | 1.00 | 28.84 |
| 4113 | O | GLN | A | 293 | 81.060 | 62.747 | -4.898 | 1.00 | 29.43 |
| 4114 | N | SER | A | 294 | 79.946 | 64.002 | -3.403 | 1.00 | 28.72 |
| 4116 | CA | SER | A | 294 | 80.514 | 63.331 | -2.234 | 1.00 | 28.70 |
| 4118 | CB | SER | A | 294 | 79.948 | 63.912 | -0.930 | 1.00 | 28.50 |
| 4121 | OG | SER | A | 294 | 80.451 | 65.214 | -0.693 | 1.00 | 28.19 |
| 4123 | C | SER | A | 294 | 80.254 | 61.824 | -2.255 | 1.00 | 28.86 |
| 4124 | O | SER | A | 294 | 81.143 | 61.046 | -1.948 | 1.00 | 28.79 |
| 4125 | N | LEU | A | 295 | 79.028 | 61.428 | -2.579 | 1.00 | 29.44 |
| 4127 | CA | LEU | A | 295 | 78.666 | 60.005 | -2.650 | 1.00 | 29.79 |
| 4129 | CB | LEU | A | 295 | 77.163 | 59.818 | -2.910 | 1.00 | 29.50 |
| 4132 | CG | LEU | A | 295 | 76.184 | 60.273 | -1.815 | 1.00 | 28.59 |
| 4134 | CD1 | LEU | A | 295 | 74.747 | 60.026 | -2.249 | 1.00 | 28.94 |
| 4138 | CD2 | LEU | A | 295 | 76.473 | 59.585 | -0.493 | 1.00 | 27.92 |
| 4142 | C | LEU | A | 295 | 79.472 | 59.246 | -3.717 | 1.00 | 30.81 |
| 4143 | O | LEU | A | 295 | 79.732 | 58.062 | -3.545 | 1.00 | 30.71 |
| 4144 | N | LYS | A | 296 | 79.870 | 59.919 | -4.800 | 1.00 | 31.59 |
| 4146 | CA | LYS | A | 296 | 80.704 | 59.288 | -5.837 | 1.00 | 32.26 |
| 4148 | CB | LYS | A | 296 | 80.998 | 60.268 | -6.989 | 1.00 | 32.55 |
| 4151 | CG | LYS | A | 296 | 79.794 | 60.560 | -7.898 | 1.00 | 34.13 |
| 4154 | CD | LYS | A | 296 | 80.188 | 61.386 | -9.153 | 1.00 | 35.23 |
| 4157 | CE | LYS | A | 296 | 79.129 | 61.238 | -10.259 | 1.00 | 36.81 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 4160 | NZ | LYS | A | 296 | 79.083 | 62.387 | -11.229 | 1.00 | 37.86 |
| 4164 | C | LYS | A | 296 | 82.012 | 58.741 | -5.256 | 1.00 | 32.60 |
| 4165 | O | LYS | A | 296 | 82.471 | 57.679 | -5.650 | 1.00 | 33.03 |
| 4166 | N | GLN | A | 297 | 82.589 | 59.462 | -4.300 | 1.00 | 33.38 |
| 4168 | CA | GLN | A | 297 | 83.796 | 59.026 | -3.599 | 1.00 | 34.01 |
| 4170 | CB | GLN | A | 297 | 84.253 | 60.103 | -2.607 | 1.00 | 34.60 |
| 4173 | CG | GLN | A | 297 | 84.614 | 61.448 | -3.230 | 1.00 | 35.87 |
| 4176 | CD | GLN | A | 297 | 85.108 | 62.446 | -2.197 | 1.00 | 37.47 |
| 4177 | OE1 | GLN | A | 297 | 86.039 | 62.155 | -1.446 | 1.00 | 39.36 |
| 4178 | NE2 | GLN | A | 297 | 84.483 | 63.615 | -2.149 | 1.00 | 39.06 |
| 4181 | C | GLN | A | 297 | 83.589 | 57.715 | -2.830 | 1.00 | 34.18 |
| 4182 | O | GLN | A | 297 | 84.513 | 56.909 | -2.707 | 1.00 | 34.15 |
| 4183 | N | LEU | A | 298 | 82.385 | 57.520 | -2.294 | 1.00 | 33.99 |
| 4185 | CA | LEU | A | 298 | 82.047 | 56.287 | -1.591 | 1.00 | 34.26 |
| 4187 | CB | LEU | A | 298 | 80.849 | 56.509 | -0.670 | 1.00 | 33.95 |
| 4190 | CG | LEU | A | 298 | 81.061 | 57.578 | 0.398 | 1.00 | 33.40 |
| 4192 | CD1 | LEU | A | 298 | 79.805 | 57.720 | 1.223 | 1.00 | 33.09 |
| 4196 | CD2 | LEU | A | 298 | 82.269 | 57.242 | 1.274 | 1.00 | 33.91 |
| 4200 | C | LEU | A | 298 | 81.738 | 55.137 | -2.533 | 1.00 | 34.79 |
| 4201 | O | LEU | A | 298 | 82.073 | 53.989 | -2.239 | 1.00 | 34.64 |
| 4202 | N | ALA | A | 299 | 81.072 | 55.445 | -3.642 | 1.00 | 35.56 |
| 4204 | CA | ALA | A | 299 | 80.741 | 54.450 | -4.660 | 1.00 | 36.49 |
| 4206 | CB | ALA | A | 299 | 79.825 | 55.061 | -5.712 | 1.00 | 36.38 |
| 4210 | C | ALA | A | 299 | 82.012 | 53.886 | -5.311 | 1.00 | 37.32 |
| 4211 | O | ALA | A | 299 | 82.015 | 52.758 | -5.799 | 1.00 | 37.70 |
| 4212 | N | GLU | A | 300 | 83.075 | 54.690 | -5.296 | 1.00 | 38.52 |
| 4214 | CA | GLU | A | 300 | 84.421 | 54.297 | -5.744 | 1.00 | 39.54 |
| 4216 | CB | GLU | A | 300 | 85.353 | 55.513 | -5.677 | 1.00 | 39.78 |
| 4219 | CG | GLU | A | 300 | 86.404 | 55.572 | -6.767 | 1.00 | 41.97 |
| 4222 | CD | GLU | A | 300 | 86.407 | 56.897 | -7.488 | 1.00 | 43.76 |
| 4223 | OE1 | GLU | A | 300 | 86.681 | 57.915 | -6.825 | 1.00 | 46.66 |
| 4224 | OE2 | GLU | A | 300 | 86.129 | 56.921 | -8.705 | 1.00 | 45.53 |
| 4225 | C | GLU | A | 300 | 85.034 | 53.179 | -4.895 | 1.00 | 39.49 |
| 4226 | O | GLU | A | 300 | 85.883 | 52.422 | -5.363 | 1.00 | 40.00 |
| 4227 | N | GLN | A | 301 | 84.617 | 53.112 | -3.638 | 1.00 | 39.43 |
| 4229 | CA | GLN | A | 301 | 85.085 | 52.109 | -2.700 | 1.00 | 39.30 |
| 4231 | CB | GLN | A | 301 | 85.306 | 52.752 | -1.324 | 1.00 | 39.51 |
| 4234 | CG | GLN | A | 301 | 86.094 | 54.061 | -1.348 | 1.00 | 40.85 |
| 4237 | CD | GLN | A | 301 | 86.003 | 54.825 | -0.033 | 1.00 | 42.68 |
| 4238 | OE1 | GLN | A | 301 | 85.958 | 54.217 | 1.037 | 1.00 | 44.83 |
| 4239 | NE2 | GLN | A | 301 | 85.983 | 56.156 | -0.110 | 1.00 | 42.30 |
| 4242 | C | GLN | A | 301 | 84.087 | 50.944 | -2.594 | 1.00 | 38.62 |
| 4243 | O | GLN | A | 301 | 84.083 | 50.210 | -1.605 | 1.00 | 38.99 |
| 4244 | N | SER | A | 302 | 83.250 | 50.794 | -3.616 | 1.00 | 37.61 |
| 4246 | CA | SER | A | 302 | 82.260 | 49.718 | -3.721 | 1.00 | 36.98 |
| 4248 | CB | SER | A | 302 | 82.963 | 48.362 | -3.884 | 1.00 | 37.17 |
| 4251 | OG | SER | A | 302 | 83.487 | 48.241 | -5.197 | 1.00 | 38.77 |
| 4253 | C | SER | A | 302 | 81.210 | 49.685 | -2.598 | 1.00 | 35.68 |
| 4254 | O | SER | A | 302 | 80.722 | 48.617 | -2.206 | 1.00 | 35.55 |
| 4255 | N | LEU | A | 303 | 80.867 | 50.865 | -2.092 | 1.00 | 34.25 |
| 4257 | CA | LEU | A | 303 | 79.710 | 51.032 | -1.218 | 1.00 | 32.88 |
| 4259 | CB | LEU | A | 303 | 79.997 | 52.090 | -0.161 | 1.00 | 32.92 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 4262 | CG | LEU | A | 303 | 81.178 | 51.793 | 0.755 | 1.00 | 33.21 |
| 4264 | CD1 | LEU | A | 303 | 81.567 | 53.040 | 1.532 | 1.00 | 33.05 |
| 4268 | CD2 | LEU | A | 303 | 80.872 | 50.609 | 1.704 | 1.00 | 33.61 |
| 4272 | C | LEU | A | 303 | 78.507 | 51.432 | -2.074 | 1.00 | 31.66 |
| 4273 | O | LEU | A | 303 | 78.621 | 52.255 | -2.988 | 1.00 | 31.32 |
| 4274 | N | ASP | A | 304 | 77.361 | 50.827 | -1.799 | 1.00 | 30.63 |
| 4276 | CA | ASP | A | 304 | 76.127 | 51.123 | -2.528 | 1.00 | 29.60 |
| 4278 | CB | ASP | A | 304 | 75.150 | 49.956 | -2.371 | 1.00 | 29.83 |
| 4281 | CG | ASP | A | 304 | 73.911 | 50.089 | -3.251 | 1.00 | 30.98 |
| 4282 | OD1 | ASP | A | 304 | 73.673 | 51.177 | -3.843 | 1.00 | 30.78 |
| 4283 | OD2 | ASP | A | 304 | 73.117 | 49.135 | -3.407 | 1.00 | 32.78 |
| 4284 | C | ASP | A | 304 | 75.516 | 52.431 | -2.021 | 1.00 | 28.62 |
| 4285 | O | ASP | A | 304 | 74.919 | 52.474 | -0.953 | 1.00 | 27.93 |
| 4286 | N | THR | A | 305 | 75.655 | 53.496 | -2.801 | 1.00 | 27.78 |
| 4288 | CA | THR | A | 305 | 75.152 | 54.812 | -2.395 | 1.00 | 27.48 |
| 4290 | CB | THR | A | 305 | 76.121 | 55.907 | -2.850 | 1.00 | 27.79 |
| 4292 | OG1 | THR | A | 305 | 76.198 | 55.923 | -4.282 | 1.00 | 27.64 |
| 4294 | CG2 | THR | A | 305 | 77.522 | 55.612 | -2.397 | 1.00 | 27.86 |
| 4298 | C | THR | A | 305 | 73.775 | 55.130 | -2.963 | 1.00 | 26.98 |
| 4299 | O | THR | A | 305 | 73.314 | 56.269 | -2.852 | 1.00 | 26.90 |
| 4300 | N | SER | A | 306 | 73.115 | 54.136 | -3.549 | 1.00 | 25.87 |
| 4302 | CA | SER | A | 306 | 71.884 | 54.371 | -4.303 | 1.00 | 25.78 |
| 4304 | CB | SER | A | 306 | 71.469 | 53.116 | -5.083 | 1.00 | 25.66 |
| 4307 | OG | SER | A | 306 | 71.181 | 52.042 | -4.210 | 1.00 | 28.03 |
| 4309 | C | SER | A | 306 | 70.718 | 54.922 | -3.460 | 1.00 | 24.86 |
| 4310 | O | SER | A | 306 | 69.989 | 55.799 | -3.922 | 1.00 | 24.04 |
| 4311 | N | ALA | A | 307 | 70.538 | 54.423 | -2.237 | 1.00 | 24.31 |
| 4313 | CA | ALA | A | 307 | 69.491 | 54.957 | -1.356 | 1.00 | 23.85 |
| 4315 | CB | ALA | A | 307 | 69.266 | 54.058 | -0.138 | 1.00 | 23.74 |
| 4319 | C | ALA | A | 307 | 69.813 | 56.402 | -0.925 | 1.00 | 23.51 |
| 4320 | O | ALA | A | 307 | 68.927 | 57.234 | -0.865 | 1.00 | 22.49 |
| 4321 | N | LEU | A | 308 | 71.082 | 56.696 | -0.670 | 1.00 | 23.59 |
| 4323 | CA | LEU | A | 308 | 71.476 | 58.050 | -0.254 | 1.00 | 24.04 |
| 4325 | CB | LEU | A | 308 | 72.893 | 58.059 | 0.321 | 1.00 | 23.68 |
| 4328 | CG | LEU | A | 308 | 73.047 | 57.380 | 1.677 | 1.00 | 24.07 |
| 4330 | CD1 | LEU | A | 308 | 74.495 | 57.511 | 2.165 | 1.00 | 25.59 |
| 4334 | CD2 | LEU | A | 308 | 72.085 | 57.972 | 2.680 | 1.00 | 24.26 |
| 4338 | C | LEU | A | 308 | 71.375 | 59.070 | -1.370 | 1.00 | 24.05 |
| 4339 | O | LEU | A | 308 | 71.128 | 60.238 | -1.104 | 1.00 | 24.30 |
| 4340 | N | GLU | A | 309 | 71.575 | 58.648 | -2.614 | 1.00 | 24.92 |
| 4342 | CA | GLU | A | 309 | 71.455 | 59.578 | -3.734 | 1.00 | 25.79 |
| 4344 | CB | GLU | A | 309 | 72.238 | 59.158 | -4.988 | 1.00 | 26.38 |
| 4347 | CG | GLU | A | 309 | 72.152 | 57.732 | -5.448 | 1.00 | 28.99 |
| 4350 | CD | GLU | A | 309 | 73.344 | 57.345 | -6.333 | 1.00 | 31.29 |
| 4351 | OE1 | GLU | A | 309 | 73.673 | 58.127 | -7.247 | 1.00 | 31.21 |
| 4352 | OE2 | GLU | A | 309 | 73.966 | 56.274 | -6.098 | 1.00 | 33.39 |
| 4353 | C | GLU | A | 309 | 69.982 | 59.834 | -4.045 | 1.00 | 25.52 |
| 4354 | O | GLU | A | 309 | 69.605 | 60.961 | -4.347 | 1.00 | 25.13 |
| 4355 | N | ALA | A | 310 | 69.152 | 58.797 | -3.927 | 1.00 | 25.73 |
| 4357 | CA | ALA | A | 310 | 67.709 | 58.953 | -4.149 | 1.00 | 25.33 |
| 4359 | CB | ALA | A | 310 | 67.020 | 57.609 | -4.201 | 1.00 | 25.75 |
| 4363 | C | ALA | A | 310 | 67.099 | 59.830 | -3.059 | 1.00 | 25.32 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 4364 | O | ALA | A | 310 | 66.202 | 60.633 | -3.328 | 1.00 | 24.76 |
| 4365 | N | LEU | A | 311 | 67.591 | 59.677 | -1.828 | 1.00 | 25.18 |
| 4367 | CA | LEU | A | 311 | 67.117 | 60.499 | -0.711 | 1.00 | 25.23 |
| 4369 | CB | LEU | A | 311 | 67.707 | 59.988 | 0.608 | 1.00 | 25.28 |
| 4372 | CG | LEU | A | 311 | 67.209 | 60.548 | 1.945 | 1.00 | 27.23 |
| 4374 | CD1 | LEU | A | 311 | 67.788 | 61.919 | 2.199 | 1.00 | 29.43 |
| 4378 | CD2 | LEU | A | 311 | 65.687 | 60.595 | 2.012 | 1.00 | 28.69 |
| 4382 | C | LEU | A | 311 | 67.520 | 61.954 | -0.959 | 1.00 | 24.32 |
| 4383 | O | LEU | A | 311 | 66.719 | 62.872 | -0.780 | 1.00 | 23.70 |
| 4384 | N | ALA | A | 312 | 68.758 | 62.146 | -1.399 | 1.00 | 23.80 |
| 4386 | CA | ALA | A | 312 | 69.282 | 63.481 | -1.672 | 1.00 | 24.14 |
| 4388 | CB | ALA | A | 312 | 70.733 | 63.405 | -2.153 | 1.00 | 24.17 |
| 4392 | C | ALA | A | 312 | 68.410 | 64.218 | -2.687 | 1.00 | 24.07 |
| 4393 | O | ALA | A | 312 | 68.063 | 65.382 | -2.480 | 1.00 | 23.69 |
| 4394 | N | ASP | A | 313 | 68.027 | 63.538 | -3.761 | 1.00 | 24.24 |
| 4396 | CA | ASP | A | 313 | 67.146 | 64.143 | -4.772 | 1.00 | 24.99 |
| 4398 | CB | ASP | A | 313 | 67.015 | 63.231 | -5.990 | 1.00 | 25.46 |
| 4401 | CG | ASP | A | 313 | 68.259 | 63.225 | -6.840 | 1.00 | 27.73 |
| 4402 | OD1 | ASP | A | 313 | 68.311 | 62.445 | -7.819 | 1.00 | 32.11 |
| 4403 | OD2 | ASP | A | 313 | 69.231 | 63.968 | -6.614 | 1.00 | 30.06 |
| 4404 | C | ASP | A | 313 | 65.751 | 64.427 | -4.242 | 1.00 | 24.15 |
| 4405 | O | ASP | A | 313 | 65.146 | 65.464 | -4.565 | 1.00 | 23.53 |
| 4406 | N | TYR | A | 314 | 65.233 | 63.497 | -3.445 | 1.00 | 23.64 |
| 4408 | CA | TYR | A | 314 | 63.890 | 63.636 | -2.889 | 1.00 | 23.49 |
| 4410 | CB | TYR | A | 314 | 63.465 | 62.369 | -2.150 | 1.00 | 23.53 |
| 4413 | CG | TYR | A | 314 | 62.066 | 62.432 | -1.543 | 1.00 | 23.83 |
| 4414 | CD1 | TYR | A | 314 | 61.882 | 62.358 | -0.171 | 1.00 | 24.83 |
| 4416 | CE1 | TYR | A | 314 | 60.607 | 62.425 | 0.392 | 1.00 | 25.12 |
| 4418 | CZ | TYR | A | 314 | 59.501 | 62.553 | -0.424 | 1.00 | 26.00 |
| 4419 | OH | TYR | A | 314 | 58.239 | 62.602 | 0.134 | 1.00 | 26.70 |
| 4421 | CE2 | TYR | A | 314 | 59.660 | 62.622 | -1.798 | 1.00 | 25.30 |
| 4423 | CD2 | TYR | A | 314 | 60.939 | 62.568 | -2.344 | 1.00 | 23.99 |
| 4425 | C | TYR | A | 314 | 63.824 | 64.844 | -1.957 | 1.00 | 23.57 |
| 4426 | O | TYR | A | 314 | 62.829 | 65.529 | -1.919 | 1.00 | 22.72 |
| 4427 | N | ILE | A | 315 | 64.902 | 65.112 | -1.229 | 1.00 | 24.12 |
| 4429 | CA | ILE | A | 315 | 64.949 | 66.247 | -0.301 | 1.00 | 24.93 |
| 4431 | CB | ILE | A | 315 | 66.333 | 66.304 | 0.411 | 1.00 | 24.90 |
| 4433 | CG1 | ILE | A | 315 | 66.333 | 65.285 | 1.553 | 1.00 | 25.34 |
| 4436 | CD1 | ILE | A | 315 | 67.675 | 65.077 | 2.197 | 1.00 | 27.41 |
| 4440 | CG2 | ILE | A | 315 | 66.639 | 67.710 | 0.943 | 1.00 | 25.11 |
| 4444 | C | ILE | A | 315 | 64.575 | 67.576 | -0.977 | 1.00 | 25.41 |
| 4445 | O | ILE | A | 315 | 64.017 | 68.468 | -0.326 | 1.00 | 25.21 |
| 4446 | N | ILE | A | 316 | 64.848 | 67.702 | -2.274 | 1.00 | 25.98 |
| 4448 | CA | ILE | A | 316 | 64.481 | 68.928 | -3.003 | 1.00 | 26.46 |
| 4450 | CB | ILE | A | 316 | 65.736 | 69.586 | -3.590 | 1.00 | 26.50 |
| 4452 | CG1 | ILE | A | 316 | 66.349 | 68.722 | -4.700 | 1.00 | 26.76 |
| 4455 | CD1 | ILE | A | 316 | 67.350 | 69.472 | -5.530 | 1.00 | 27.27 |
| 4459 | CG2 | ILE | A | 316 | 66.729 | 69.819 | -2.491 | 1.00 | 26.11 |
| 4463 | C | ILE | A | 316 | 63.393 | 68.781 | -4.066 | 1.00 | 26.91 |
| 4464 | O | ILE | A | 316 | 62.930 | 69.779 | -4.622 | 1.00 | 26.80 |
| 4465 | N | GLN | A | 317 | 62.982 | 67.543 | -4.337 | 1.00 | 26.94 |
| 4467 | CA | GLN | A | 317 | 61.911 | 67.267 | -5.284 | 1.00 | 27.25 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 4469 | CB | GLN | A | 317 | 62.217 | 65.999 | -6.089 | 1.00 | 27.44 |
| 4472 | CG | GLN | A | 317 | 63.241 | 66.219 | -7.186 | 1.00 | 30.05 |
| 4475 | CD | GLN | A | 317 | 63.720 | 64.922 | -7.830 | 1.00 | 33.37 |
| 4476 | OE1 | GLN | A | 317 | 64.730 | 64.920 | -8.521 | 1.00 | 36.33 |
| 4477 | NE2 | GLN | A | 317 | 62.999 | 63.828 | -7.606 | 1.00 | 34.01 |
| 4480 | C | GLN | A | 317 | 60.573 | 67.102 | -4.575 | 1.00 | 26.71 |
| 4481 | O | GLN | A | 317 | 59.514 | 67.225 | -5.193 | 1.00 | 27.01 |
| 4482 | N | ARG | A | 318 | 60.620 | 66.825 | -3.280 | 1.00 | 26.09 |
| 4484 | CA | ARG | A | 318 | 59.418 | 66.570 | -2.503 | 1.00 | 25.94 |
| 4486 | CB | ARG | A | 318 | 59.774 | 66.077 | -1.098 | 1.00 | 25.87 |
| 4489 | CG | ARG | A | 318 | 60.382 | 67.160 | -0.225 | 1.00 | 25.06 |
| 4492 | CD | ARG | A | 318 | 61.211 | 66.630 | 0.914 | 1.00 | 23.99 |
| 4495 | NE | ARG | A | 318 | 61.963 | 67.704 | 1.555 | 1.00 | 22.64 |
| 4497 | CZ | ARG | A | 318 | 61.503 | 68.481 | 2.528 | 1.00 | 19.61 |
| 4498 | NH1 | ARG | A | 318 | 62.286 | 69.429 | 3.025 | 1.00 | 20.15 |
| 4501 | NH2 | ARG | A | 318 | 60.289 | 68.325 | 3.008 | 1.00 | 19.15 |
| 4504 | C | ARG | A | 318 | 58.558 | 67.817 | -2.386 | 1.00 | 26.24 |
| 4505 | O | ARG | A | 318 | 59.053 | 68.938 | -2.448 | 1.00 | 25.48 |
| 4506 | N | ASN | A | 319 | 57.269 | 67.601 | -2.191 | 1.00 | 26.97 |
| 4508 | CA | ASN | A | 319 | 56.321 | 68.702 | -2.054 | 1.00 | 28.44 |
| 4510 | CB | ASN | A | 319 | 55.255 | 68.594 | -3.128 | 1.00 | 28.90 |
| 4513 | CG | ASN | A | 319 | 55.820 | 68.829 | -4.487 | 1.00 | 31.25 |
| 4514 | OD1 | ASN | A | 319 | 56.328 | 69.921 | -4.771 | 1.00 | 36.72 |
| 4515 | ND2 | ASN | A | 319 | 55.782 | 67.807 | -5.337 | 1.00 | 35.16 |
| 4518 | C | ASN | A | 319 | 55.711 | 68.729 | -0.676 | 1.00 | 28.47 |
| 4519 | O | ASN | A | 319 | 54.731 | 69.426 | -0.440 | 1.00 | 28.00 |
| 4520 | N | LYS | A | 320 | 56.326 | 67.972 | 0.234 | 1.00 | 29.44 |
| 4522 | CA | LYS | A | 320 | 55.925 | 67.944 | 1.642 | 1.00 | 30.19 |
| 4524 | CB | LYS | A | 320 | 54.722 | 67.029 | 1.835 | 1.00 | 30.27 |
| 4527 | CG | LYS | A | 320 | 54.874 | 65.638 | 1.202 | 1.00 | 32.14 |
| 4530 | CD | LYS | A | 320 | 54.635 | 64.498 | 2.180 | 1.00 | 34.17 |
| 4533 | CE | LYS | A | 320 | 53.660 | 63.459 | 1.652 | 1.00 | 35.54 |
| 4536 | NZ | LYS | A | 320 | 54.228 | 62.656 | 0.542 | 1.00 | 36.19 |
| 4540 | C | LYS | A | 320 | 57.081 | 67.487 | 2.528 | 1.00 | 30.38 |
| 4541 | O | LYS | A | 320 | 56.992 | 67.504 | 3.759 | 1.00 | 30.94 |
| 4542 | OXT | LYS | A | 320 | 58.130 | 67.081 | 2.028 | 1.00 | 30.00 |
| 4543 | N | ASP | B | 23 | 19.060 | 6.498 | -16.010 | 1.00 | 36.37 |
| 4545 | CA | ASP | B | 23 | 17.827 | 7.340 | -15.968 | 1.00 | 36.07 |
| 4547 | CB | ASP | B | 23 | 16.585 | 6.454 | -15.910 | 1.00 | 36.75 |
| 4550 | CG | ASP | B | 23 | 15.301 | 7.258 | -15.889 | 1.00 | 38.21 |
| 4551 | OD1 | ASP | B | 23 | 15.288 | 8.356 | -16.476 | 1.00 | 42.09 |
| 4552 | OD2 | ASP | B | 23 | 14.258 | 6.882 | -15.321 | 1.00 | 41.73 |
| 4553 | C | ASP | B | 23 | 17.853 | 8.266 | -14.742 | 1.00 | 35.62 |
| 4554 | O | ASP | B | 23 | 17.713 | 7.800 | -13.603 | 1.00 | 35.09 |
| 4557 | N | PHE | B | 24 | 18.002 | 9.572 | -14.969 | 1.00 | 34.42 |
| 4559 | CA | PHE | B | 24 | 18.233 | 10.472 | -13.845 | 1.00 | 33.65 |
| 4561 | CB | PHE | B | 24 | 18.831 | 11.812 | -14.264 | 1.00 | 33.54 |
| 4564 | CG | PHE | B | 24 | 19.286 | 12.629 | -13.097 | 1.00 | 32.06 |
| 4565 | CD1 | PHE | B | 24 | 20.342 | 12.202 | -12.312 | 1.00 | 31.59 |
| 4567 | CE1 | PHE | B | 24 | 20.747 | 12.940 | -11.217 | 1.00 | 31.53 |
| 4569 | CZ | PHE | B | 24 | 20.080 | 14.100 | -10.888 | 1.00 | 30.24 |
| 4571 | CE2 | PHE | B | 24 | 19.029 | 14.516 | -11.638 | 1.00 | 31.16 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 4573 | CD2 | PHE | B | 24 | 18.621 | 13.779 | -12.739 | 1.00 | 32.52 |
| 4575 | C | PHE | B | 24 | 17.015 | 10.695 | -12.946 | 1.00 | 33.05 |
| 4576 | O | PHE | B | 24 | 17.179 | 10.672 | -11.738 | 1.00 | 32.55 |
| 4577 | N | PRO | B | 25 | 15.817 | 10.901 | -13.503 | 1.00 | 32.85 |
| 4578 | CA | PRO | B | 25 | 14.606 | 11.056 | -12.680 | 1.00 | 32.66 |
| 4580 | CB | PRO | B | 25 | 13.497 | 11.261 | -13.722 | 1.00 | 32.79 |
| 4583 | CG | PRO | B | 25 | 14.213 | 11.795 | -14.914 | 1.00 | 33.05 |
| 4586 | CD | PRO | B | 25 | 15.508 | 11.051 | -14.936 | 1.00 | 32.96 |
| 4589 | C | PRO | B | 25 | 14.285 | 9.869 | -11.768 | 1.00 | 32.36 |
| 4590 | O | PRO | B | 25 | 13.759 | 10.093 | -10.685 | 1.00 | 31.80 |
| 4591 | N | GLN | B | 26 | 14.594 | 8.643 | -12.190 | 1.00 | 31.98 |
| 4593 | CA | GLN | B | 26 | 14.399 | 7.478 | -11.329 | 1.00 | 32.12 |
| 4595 | CB | GLN | B | 26 | 14.282 | 6.175 | -12.145 | 1.00 | 32.62 |
| 4598 | CG | GLN | B | 26 | 12.872 | 5.922 | -12.758 | 1.00 | 35.79 |
| 4601 | CD | GLN | B | 26 | 11.784 | 5.507 | -11.736 | 1.00 | 38.90 |
| 4602 | OE1 | GLN | B | 26 | 11.382 | 4.327 | -11.677 | 1.00 | 40.51 |
| 4603 | NE2 | GLN | B | 26 | 11.292 | 6.479 | -10.956 | 1.00 | 40.37 |
| 4606 | C | GLN | B | 26 | 15.524 | 7.368 | -10.279 | 1.00 | 30.90 |
| 4607 | O | GLN | B | 26 | 15.304 | 6.829 | -9.213 | 1.00 | 30.46 |
| 4608 | N | GLN | B | 27 | 16.715 | 7.872 | -10.583 | 1.00 | 30.18 |
| 4610 | CA | GLN | B | 27 | 17.778 | 7.963 | -9.575 | 1.00 | 30.30 |
| 4612 | CB | GLN | B | 27 | 19.108 | 8.421 | -10.180 | 1.00 | 30.56 |
| 4615 | CG | GLN | B | 27 | 19.929 | 7.310 | -10.799 | 1.00 | 33.30 |
| 4618 | CD | GLN | B | 27 | 20.971 | 6.745 | -9.843 | 1.00 | 36.37 |
| 4619 | OE1 | GLN | B | 27 | 21.903 | 7.457 | -9.441 | 1.00 | 39.14 |
| 4620 | NE2 | GLN | B | 27 | 20.822 | 5.474 | -9.479 | 1.00 | 36.91 |
| 4623 | C | GLN | B | 27 | 17.364 | 8.924 | -8.464 | 1.00 | 29.14 |
| 4624 | O | GLN | B | 27 | 17.509 | 8.604 | -7.285 | 1.00 | 29.47 |
| 4625 | N | LEU | B | 28 | 16.838 | 10.086 | -8.841 | 1.00 | 27.84 |
| 4627 | CA | LEU | B | 28 | 16.384 | 11.074 | -7.864 | 1.00 | 27.57 |
| 4629 | CB | LEU | B | 28 | 15.793 | 12.309 | -8.546 | 1.00 | 27.88 |
| 4632 | CG | LEU | B | 28 | 16.740 | 13.324 | -9.180 | 1.00 | 28.18 |
| 4634 | CD1 | LEU | B | 28 | 15.884 | 14.370 | -9.884 | 1.00 | 28.62 |
| 4638 | CD2 | LEU | B | 28 | 17.667 | 13.973 | -8.145 | 1.00 | 28.38 |
| 4642 | C | LEU | B | 28 | 15.317 | 10.478 | -6.961 | 1.00 | 27.38 |
| 4643 | O | LEU | B | 28 | 15.364 | 10.643 | -5.741 | 1.00 | 26.09 |
| 4644 | N | GLU | B | 29 | 14.358 | 9.786 | -7.573 | 1.00 | 27.02 |
| 4646 | CA | GLU | B | 29 | 13.207 | 9.269 | -6.847 | 1.00 | 27.65 |
| 4648 | CB | GLU | B | 29 | 12.098 | 8.855 | -7.825 | 1.00 | 28.49 |
| 4651 | CG | GLU | B | 29 | 11.022 | 7.981 | -7.212 | 1.00 | 32.02 |
| 4654 | CD | GLU | B | 29 | 9.646 | 8.256 | -7.782 | 1.00 | 37.15 |
| 4655 | OE1 | GLU | B | 29 | 9.109 | 9.364 | -7.545 | 1.00 | 42.58 |
| 4656 | OE2 | GLU | B | 29 | 9.100 | 7.363 | -8.463 | 1.00 | 41.15 |
| 4657 | C | GLU | B | 29 | 13.618 | 8.112 | -5.938 | 1.00 | 26.50 |
| 4658 | O | GLU | B | 29 | 13.115 | 8.008 | -4.823 | 1.00 | 26.62 |
| 4659 | N | ALA | B | 30 | 14.513 | 7.250 | -6.421 | 1.00 | 25.43 |
| 4661 | CA | ALA | B | 30 | 15.092 | 6.179 | -5.610 | 1.00 | 24.85 |
| 4663 | CB | ALA | B | 30 | 16.021 | 5.297 | -6.443 | 1.00 | 24.98 |
| 4667 | C | ALA | B | 30 | 15.864 | 6.765 | -4.421 | 1.00 | 24.65 |
| 4668 | O | ALA | B | 30 | 15.827 | 6.211 | -3.318 | 1.00 | 23.25 |
| 4669 | N | CYS | B | 31 | 16.556 | 7.885 | -4.650 | 1.00 | 24.00 |
| 4671 | CA | CYS | B | 31 | 17.315 | 8.544 | -3.589 | 1.00 | 23.64 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 4673 | CB | CYS | B | 31 | 18.217 | 9.650 | -4.152 | 1.00 | 23.72 |
| 4676 | SG | CYS | B | 31 | 19.117 | 10.582 | -2.885 | 1.00 | 22.22 |
| 4677 | C | CYS | B | 31 | 16.374 | 9.096 | -2.524 | 1.00 | 23.27 |
| 4678 | O | CYS | B | 31 | 16.578 | 8.876 | -1.336 | 1.00 | 23.22 |
| 4679 | N | VAL | B | 32 | 15.323 | 9.779 | -2.945 | 1.00 | 23.25 |
| 4681 | CA | VAL | B | 32 | 14.334 | 10.280 | -2.006 | 1.00 | 23.43 |
| 4683 | CB | VAL | B | 32 | 13.175 | 10.997 | -2.725 | 1.00 | 23.51 |
| 4685 | CG1 | VAL | B | 32 | 12.005 | 11.220 | -1.804 | 1.00 | 24.68 |
| 4689 | CG2 | VAL | B | 32 | 13.650 | 12.324 | -3.276 | 1.00 | 23.07 |
| 4693 | C | VAL | B | 32 | 13.811 | 9.132 | -1.138 | 1.00 | 23.73 |
| 4694 | O | VAL | B | 32 | 13.641 | 9.300 | 0.067 | 1.00 | 23.38 |
| 4695 | N | LYS | B | 33 | 13.581 | 7.964 | -1.737 | 1.00 | 23.54 |
| 4697 | CA | LYS | B | 33 | 13.012 | 6.852 | -0.972 | 1.00 | 24.03 |
| 4699 | CB | LYS | B | 33 | 12.440 | 5.765 | -1.891 | 1.00 | 24.27 |
| 4702 | CG | LYS | B | 33 | 10.995 | 6.086 | -2.256 | 1.00 | 27.21 |
| 4705 | CD | LYS | B | 33 | 10.544 | 5.567 | -3.606 | 1.00 | 31.82 |
| 4708 | CE | LYS | B | 33 | 9.032 | 5.811 | -3.762 | 1.00 | 33.94 |
| 4711 | NZ | LYS | B | 33 | 8.488 | 5.279 | -5.045 | 1.00 | 37.62 |
| 4715 | C | LYS | B | 33 | 14.026 | 6.287 | -0.004 | 1.00 | 22.89 |
| 4716 | O | LYS | B | 33 | 13.699 | 6.017 | 1.145 | 1.00 | 23.39 |
| 4717 | N | GLN | B | 34 | 15.257 | 6.124 | -0.468 | 1.00 | 22.27 |
| 4719 | CA | GLN | B | 34 | 16.335 | 5.645 | 0.380 | 1.00 | 21.89 |
| 4721 | CB | GLN | B | 34 | 17.623 | 5.496 | -0.423 | 1.00 | 21.61 |
| 4724 | CG | GLN | B | 34 | 18.810 | 4.946 | 0.352 | 1.00 | 21.80 |
| 4727 | CD | GLN | B | 34 | 18.683 | 3.471 | 0.705 | 1.00 | 23.69 |
| 4728 | OE1 | GLN | B | 34 | 19.316 | 2.999 | 1.657 | 1.00 | 25.82 |
| 4729 | NE2 | GLN | B | 34 | 17.882 | 2.742 | -0.054 | 1.00 | 22.57 |
| 4732 | C | GLN | B | 34 | 16.518 | 6.604 | 1.561 | 1.00 | 21.61 |
| 4733 | O | GLN | B | 34 | 16.596 | 6.163 | 2.704 | 1.00 | 21.00 |
| 4734 | N | ALA | B | 35 | 16.556 | 7.906 | 1.285 | 1.00 | 21.58 |
| 4736 | CA | ALA | B | 35 | 16.835 | 8.916 | 2.323 | 1.00 | 21.82 |
| 4738 | CB | ALA | B | 35 | 17.120 | 10.295 | 1.691 | 1.00 | 21.91 |
| 4742 | C | ALA | B | 35 | 15.684 | 9.025 | 3.317 | 1.00 | 21.73 |
| 4743 | O | ALA | B | 35 | 15.897 | 9.174 | 4.508 | 1.00 | 21.94 |
| 4744 | N | ASN | B | 36 | 14.461 | 8.963 | 2.822 | 1.00 | 22.10 |
| 4746 | CA | ASN | B | 36 | 13.289 | 8.996 | 3.699 | 1.00 | 22.38 |
| 4748 | CB | ASN | B | 36 | 12.013 | 9.035 | 2.869 | 1.00 | 22.05 |
| 4751 | CG | ASN | B | 36 | 11.720 | 10.416 | 2.319 | 1.00 | 23.08 |
| 4752 | OD1 | ASN | B | 36 | 12.374 | 11.387 | 2.689 | 1.00 | 22.74 |
| 4753 | ND2 | ASN | B | 36 | 10.732 | 10.510 | 1.424 | 1.00 | 22.09 |
| 4756 | C | ASN | B | 36 | 13.237 | 7.812 | 4.655 | 1.00 | 22.64 |
| 4757 | O | ASN | B | 36 | 12.857 | 7.962 | 5.811 | 1.00 | 22.97 |
| 4758 | N | GLN | B | 37 | 13.604 | 6.637 | 4.160 | 1.00 | 22.84 |
| 4760 | CA | GLN | B | 37 | 13.624 | 5.438 | 4.978 | 1.00 | 23.34 |
| 4762 | CB | GLN | B | 37 | 13.859 | 4.210 | 4.085 | 1.00 | 23.43 |
| 4765 | CG | GLN | B | 37 | 14.118 | 2.893 | 4.795 | 1.00 | 26.33 |
| 4768 | CD | GLN | B | 37 | 14.528 | 1.795 | 3.815 | 1.00 | 28.80 |
| 4769 | OE1 | GLN | B | 37 | 15.700 | 1.679 | 3.443 | 1.00 | 33.07 |
| 4770 | NE2 | GLN | B | 37 | 13.560 | 1.007 | 3.378 | 1.00 | 32.12 |
| 4773 | C | GLN | B | 37 | 14.720 | 5.582 | 6.039 | 1.00 | 23.12 |
| 4774 | O | GLN | B | 37 | 14.542 | 5.183 | 7.178 | 1.00 | 23.43 |
| 4775 | N | ALA | B | 38 | 15.855 | 6.146 | 5.653 | 1.00 | 22.32 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 4777 | CA | ALA | B | 38 | 16.974 | 6.318 | 6.569 | 1.00 | 22.90 |
| 4779 | CB | ALA | B | 38 | 18.199 | 6.814 | 5.818 | 1.00 | 22.55 |
| 4783 | C | ALA | B | 38 | 16.590 | 7.296 | 7.679 | 1.00 | 22.66 |
| 4784 | O | ALA | B | 38 | 16.750 | 6.992 | 8.861 | 1.00 | 22.59 |
| 4785 | N | LEU | B | 39 | 16.069 | 8.457 | 7.288 | 1.00 | 22.88 |
| 4787 | CA | LEU | B | 39 | 15.603 | 9.462 | 8.244 | 1.00 | 23.19 |
| 4789 | CB | LEU | B | 39 | 14.980 | 10.661 | 7.521 | 1.00 | 23.23 |
| 4792 | CG | LEU | B | 39 | 15.948 | 11.654 | 6.869 | 1.00 | 24.18 |
| 4794 | CD1 | LEU | B | 39 | 15.253 | 12.531 | 5.850 | 1.00 | 25.04 |
| 4798 | CD2 | LEU | B | 39 | 16.610 | 12.528 | 7.925 | 1.00 | 25.95 |
| 4802 | C | LEU | B | 39 | 14.565 | 8.869 | 9.206 | 1.00 | 23.67 |
| 4803 | O | LEU | B | 39 | 14.665 | 9.037 | 10.415 | 1.00 | 22.94 |
| 4804 | N | SER | B | 40 | 13.573 | 8.180 | 8.654 | 1.00 | 24.43 |
| 4806 | CA | SER | B | 40 | 12.506 | 7.580 | 9.458 | 1.00 | 25.35 |
| 4808 | CB | SER | B | 40 | 11.490 | 6.887 | 8.551 | 1.00 | 25.51 |
| 4811 | OG | SER | B | 40 | 10.877 | 7.830 | 7.706 | 1.00 | 26.80 |
| 4813 | C | SER | B | 40 | 13.043 | 6.579 | 10.487 | 1.00 | 25.98 |
| 4814 | O | SER | B | 40 | 12.547 | 6.525 | 11.610 | 1.00 | 26.04 |
| 4815 | N | ARG | B | 41 | 14.062 | 5.813 | 10.094 | 1.00 | 26.60 |
| 4817 | CA | ARG | B | 41 | 14.700 | 4.820 | 10.962 | 1.00 | 27.70 |
| 4819 | CB | ARG | B | 41 | 15.743 | 3.993 | 10.185 | 1.00 | 28.27 |
| 4822 | CG | ARG | B | 41 | 15.205 | 2.761 | 9.484 | 1.00 | 31.67 |
| 4825 | CD | ARG | B | 41 | 16.207 | 1.605 | 9.357 | 1.00 | 34.70 |
| 4828 | NE | ARG | B | 41 | 17.593 | 2.056 | 9.140 | 1.00 | 36.06 |
| 4830 | CZ | ARG | B | 41 | 18.083 | 2.498 | 7.984 | 1.00 | 33.83 |
| 4831 | NH1 | ARG | B | 41 | 17.320 | 2.570 | 6.914 | 1.00 | 34.48 |
| 4834 | NH2 | ARG | B | 41 | 19.354 | 2.876 | 7.903 | 1.00 | 33.58 |
| 4837 | C | ARG | B | 41 | 15.407 | 5.464 | 12.148 | 1.00 | 27.46 |
| 4838 | O | ARG | B | 41 | 15.465 | 4.877 | 13.237 | 1.00 | 27.43 |
| 4839 | N | PHE | B | 42 | 15.967 | 6.655 | 11.926 | 1.00 | 27.31 |
| 4841 | CA | PHE | B | 42 | 16.692 | 7.373 | 12.965 | 1.00 | 26.91 |
| 4843 | CB | PHE | B | 42 | 17.758 | 8.289 | 12.356 | 1.00 | 26.72 |
| 4846 | CG | PHE | B | 42 | 18.835 | 7.547 | 11.623 | 1.00 | 24.89 |
| 4847 | CD1 | PHE | B | 42 | 19.206 | 7.916 | 10.343 | 1.00 | 22.57 |
| 4849 | CE1 | PHE | B | 42 | 20.201 | 7.220 | 9.656 | 1.00 | 22.79 |
| 4851 | CZ | PHE | B | 42 | 20.845 | 6.150 | 10.267 | 1.00 | 23.00 |
| 4853 | CE2 | PHE | B | 42 | 20.493 | 5.777 | 11.546 | 1.00 | 24.18 |
| 4855 | CD2 | PHE | B | 42 | 19.488 | 6.473 | 12.224 | 1.00 | 24.53 |
| 4857 | C | PHE | B | 42 | 15.763 | 8.164 | 13.851 | 1.00 | 27.56 |
| 4858 | O | PHE | B | 42 | 16.136 | 8.505 | 14.964 | 1.00 | 28.14 |
| 4859 | N | ILE | B | 43 | 14.563 | 8.457 | 13.357 | 1.00 | 28.06 |
| 4861 | CA | ILE | B | 43 | 13.570 | 9.208 | 14.113 | 1.00 | 29.01 |
| 4863 | CB | ILE | B | 43 | 12.677 | 10.054 | 13.160 | 1.00 | 29.24 |
| 4865 | CG1 | ILE | B | 43 | 13.470 | 11.240 | 12.608 | 1.00 | 28.43 |
| 4868 | CD1 | ILE | B | 43 | 12.767 | 12.003 | 11.524 | 1.00 | 29.06 |
| 4872 | CG2 | ILE | B | 43 | 11.412 | 10.552 | 13.876 | 1.00 | 30.14 |
| 4876 | C | ILE | B | 43 | 12.719 | 8.257 | 14.959 | 1.00 | 29.75 |
| 4877 | O | ILE | B | 43 | 12.120 | 8.678 | 15.948 | 1.00 | 30.10 |
| 4878 | N | ALA | B | 44 | 12.698 | 6.977 | 14.580 | 1.00 | 30.36 |
| 4880 | CA | ALA | B | 44 | 11.784 | 5.995 | 15.172 | 1.00 | 30.63 |
| 4882 | CB | ALA | B | 44 | 11.849 | 4.666 | 14.409 | 1.00 | 30.80 |
| 4886 | C | ALA | B | 44 | 12.021 | 5.762 | 16.651 | 1.00 | 30.90 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 4887 | O | ALA | B | 44 | 11.052 | 5.739 | 17.415 | 1.00 | 31.31 |
| 4888 | N | PRO | B | 45 | 13.278 | 5.595 | 17.074 | 1.00 | 31.28 |
| 4889 | CA | PRO | B | 45 | 13.573 | 5.370 | 18.494 | 1.00 | 31.54 |
| 4891 | CB | PRO | B | 45 | 15.045 | 4.922 | 18.489 | 1.00 | 31.77 |
| 4894 | CG | PRO | B | 45 | 15.425 | 4.741 | 17.062 | 1.00 | 32.00 |
| 4897 | CD | PRO | B | 45 | 14.512 | 5.594 | 16.270 | 1.00 | 31.28 |
| 4900 | C | PRO | B | 45 | 13.423 | 6.610 | 19.377 | 1.00 | 31.62 |
| 4901 | O | PRO | B | 45 | 13.551 | 6.466 | 20.594 | 1.00 | 32.39 |
| 4902 | N | LEU | B | 46 | 13.184 | 7.790 | 18.794 | 1.00 | 30.70 |
| 4904 | CA | LEU | B | 46 | 13.053 | 9.012 | 19.575 | 1.00 | 30.07 |
| 4906 | CB | LEU | B | 46 | 12.980 | 10.253 | 18.670 | 1.00 | 30.11 |
| 4909 | CG | LEU | B | 46 | 14.228 | 10.593 | 17.836 | 1.00 | 30.37 |
| 4911 | CD1 | LEU | B | 46 | 13.985 | 11.886 | 17.056 | 1.00 | 30.25 |
| 4915 | CD2 | LEU | B | 46 | 15.502 | 10.691 | 18.687 | 1.00 | 30.52 |
| 4919 | C | LEU | B | 46 | 11.801 | 8.963 | 20.448 | 1.00 | 29.37 |
| 4920 | O | LEU | B | 46 | 10.747 | 8.494 | 20.005 | 1.00 | 29.73 |
| 4921 | N | PRO | B | 47 | 11.903 | 9.477 | 21.669 | 1.00 | 28.40 |
| 4922 | CA | PRO | B | 47 | 10.738 | 9.551 | 22.553 | 1.00 | 28.09 |
| 4924 | CB | PRO | B | 47 | 11.355 | 9.872 | 23.921 | 1.00 | 28.24 |
| 4927 | CG | PRO | B | 47 | 12.658 | 10.565 | 23.613 | 1.00 | 28.08 |
| 4930 | CD | PRO | B | 47 | 13.115 | 10.033 | 22.301 | 1.00 | 28.09 |
| 4933 | C | PRO | B | 47 | 9.796 | 10.657 | 22.100 | 1.00 | 27.75 |
| 4934 | O | PRO | B | 47 | 10.119 | 11.411 | 21.154 | 1.00 | 26.90 |
| 4935 | N | PHE | B | 48 | 8.630 | 10.724 | 22.739 | 1.00 | 27.16 |
| 4937 | CA | PHE | B | 48 | 7.644 | 11.774 | 22.477 | 1.00 | 27.19 |
| 4939 | CB | PHE | B | 48 | 8.224 | 13.158 | 22.776 | 1.00 | 27.06 |
| 4942 | CG | PHE | B | 48 | 8.887 | 13.259 | 24.118 | 1.00 | 27.64 |
| 4943 | CD1 | PHE | B | 48 | 8.136 | 13.124 | 25.279 | 1.00 | 28.66 |
| 4945 | CE1 | PHE | B | 48 | 8.732 | 13.207 | 26.518 | 1.00 | 29.45 |
| 4947 | CZ | PHE | B | 48 | 10.096 | 13.439 | 26.617 | 1.00 | 28.49 |
| 4949 | CE2 | PHE | B | 48 | 10.863 | 13.574 | 25.475 | 1.00 | 27.66 |
| 4951 | CD2 | PHE | B | 48 | 10.260 | 13.485 | 24.226 | 1.00 | 27.57 |
| 4953 | C | PHE | B | 48 | 7.094 | 11.730 | 21.053 | 1.00 | 27.15 |
| 4954 | O | PHE | B | 48 | 6.729 | 12.755 | 20.491 | 1.00 | 26.43 |
| 4955 | N | GLN | B | 49 | 7.015 | 10.534 | 20.489 | 1.00 | 27.91 |
| 4957 | CA | GLN | B | 49 | 6.310 | 10.320 | 19.224 | 1.00 | 28.60 |
| 4959 | CB | GLN | B | 49 | 6.294 | 8.834 | 18.858 | 1.00 | 28.40 |
| 4962 | CG | GLN | B | 49 | 7.659 | 8.201 | 18.665 | 1.00 | 28.70 |
| 4965 | CD | GLN | B | 49 | 8.379 | 8.718 | 17.438 | 1.00 | 28.74 |
| 4966 | OE1 | GLN | B | 49 | 7.765 | 8.927 | 16.394 | 1.00 | 29.53 |
| 4967 | NE2 | GLN | B | 49 | 9.685 | 8.915 | 17.558 | 1.00 | 28.45 |
| 4970 | C | GLN | B | 49 | 4.868 | 10.796 | 19.363 | 1.00 | 29.43 |
| 4971 | O | GLN | B | 49 | 4.275 | 10.720 | 20.449 | 1.00 | 30.02 |
| 4972 | N | ASN | B | 50 | 4.311 | 11.291 | 18.268 | 1.00 | 30.07 |
| 4974 | CA | ASN | B | 50 | 2.942 | 11.787 | 18.226 | 1.00 | 30.82 |
| 4976 | CB | ASN | B | 50 | 1.943 | 10.631 | 18.396 | 1.00 | 31.34 |
| 4979 | CG | ASN | B | 50 | 2.264 | 9.445 | 17.492 | 1.00 | 32.36 |
| 4980 | OD1 | ASN | B | 50 | 2.338 | 9.579 | 16.261 | 1.00 | 35.83 |
| 4981 | ND2 | ASN | B | 50 | 2.480 | 8.288 | 18.096 | 1.00 | 33.67 |
| 4984 | C | ASN | B | 50 | 2.684 | 12.898 | 19.244 | 1.00 | 30.94 |
| 4985 | O | ASN | B | 50 | 1.596 | 12.983 | 19.805 | 1.00 | 31.98 |
| 4986 | N | THR | B | 51 | 3.705 | 13.716 | 19.507 | 1.00 | 30.13 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 4988 | CA | THR | B | 51 | 3.529 | 14.982 | 20.201 | 1.00 | 29.44 |
| 4990 | CB | THR | B | 51 | 4.399 | 15.055 | 21.470 | 1.00 | 29.55 |
| 4992 | OG1 | THR | B | 51 | 5.790 | 15.106 | 21.123 | 1.00 | 29.59 |
| 4994 | CG2 | THR | B | 51 | 4.249 | 13.787 | 22.313 | 1.00 | 30.13 |
| 4998 | C | THR | B | 51 | 3.901 | 16.083 | 19.216 | 1.00 | 28.76 |
| 4999 | O | THR | B | 51 | 4.574 | 15.800 | 18.231 | 1.00 | 29.08 |
| 5000 | N | PRO | B | 52 | 3.458 | 17.318 | 19.450 | 1.00 | 28.09 |
| 5001 | CA | PRO | B | 52 | 3.684 | 18.421 | 18.494 | 1.00 | 27.28 |
| 5003 | CB | PRO | B | 52 | 3.174 | 19.652 | 19.252 | 1.00 | 27.82 |
| 5006 | CG | PRO | B | 52 | 2.115 | 19.111 | 20.181 | 1.00 | 28.40 |
| 5009 | CD | PRO | B | 52 | 2.640 | 17.750 | 20.605 | 1.00 | 28.19 |
| 5012 | C | PRO | B | 52 | 5.135 | 18.643 | 18.041 | 1.00 | 26.19 |
| 5013 | O | PRO | B | 52 | 5.357 | 18.854 | 16.853 | 1.00 | 25.60 |
| 5014 | N | VAL | B | 53 | 6.100 | 18.595 | 18.957 | 1.00 | 24.76 |
| 5016 | CA | VAL | B | 53 | 7.479 | 18.902 | 18.602 | 1.00 | 23.94 |
| 5018 | CB | VAL | B | 53 | 8.365 | 19.173 | 19.859 | 1.00 | 24.25 |
| 5020 | CG1 | VAL | B | 53 | 8.593 | 17.904 | 20.684 | 1.00 | 24.46 |
| 5024 | CG2 | VAL | B | 53 | 9.678 | 19.801 | 19.452 | 1.00 | 25.37 |
| 5028 | C | VAL | B | 53 | 8.074 | 17.824 | 17.690 | 1.00 | 22.86 |
| 5029 | O | VAL | B | 53 | 8.719 | 18.150 | 16.704 | 1.00 | 21.98 |
| 5030 | N | VAL | B | 54 | 7.822 | 16.549 | 17.991 | 1.00 | 22.17 |
| 5032 | CA | VAL | B | 54 | 8.303 | 15.456 | 17.145 | 1.00 | 22.05 |
| 5034 | CB | VAL | B | 54 | 8.227 | 14.101 | 17.872 | 1.00 | 22.22 |
| 5036 | CG1 | VAL | B | 54 | 8.620 | 12.960 | 16.951 | 1.00 | 22.38 |
| 5040 | CG2 | VAL | B | 54 | 9.132 | 14.128 | 19.090 | 1.00 | 22.62 |
| 5044 | C | VAL | B | 54 | 7.547 | 15.414 | 15.816 | 1.00 | 22.15 |
| 5045 | O | VAL | B | 54 | 8.108 | 15.076 | 14.775 | 1.00 | 21.53 |
| 5046 | N | GLU | B | 55 | 6.273 | 15.760 | 15.844 | 1.00 | 22.30 |
| 5048 | CA | GLU | B | 55 | 5.501 | 15.839 | 14.612 | 1.00 | 23.31 |
| 5050 | CB | GLU | B | 55 | 4.020 | 16.062 | 14.906 | 1.00 | 23.97 |
| 5053 | CG | GLU | B | 55 | 3.349 | 14.847 | 15.529 | 1.00 | 27.97 |
| 5056 | CD | GLU | B | 55 | 1.902 | 15.107 | 15.899 | 1.00 | 32.93 |
| 5057 | OE1 | GLU | B | 55 | 1.410 | 16.237 | 15.650 | 1.00 | 37.74 |
| 5058 | OE2 | GLU | B | 55 | 1.263 | 14.182 | 16.446 | 1.00 | 36.88 |
| 5059 | C | GLU | B | 55 | 6.023 | 16.965 | 13.727 | 1.00 | 22.40 |
| 5060 | O | GLU | B | 55 | 6.016 | 16.837 | 12.516 | 1.00 | 21.26 |
| 5061 | N | THR | B | 56 | 6.497 | 18.044 | 14.344 | 1.00 | 21.39 |
| 5063 | CA | THR | B | 56 | 7.105 | 19.143 | 13.607 | 1.00 | 21.78 |
| 5065 | CB | THR | B | 56 | 7.382 | 20.353 | 14.534 | 1.00 | 22.24 |
| 5067 | OG1 | THR | B | 56 | 6.174 | 20.767 | 15.191 | 1.00 | 21.33 |
| 5069 | CG2 | THR | B | 56 | 7.803 | 21.573 | 13.727 | 1.00 | 22.96 |
| 5073 | C | THR | B | 56 | 8.406 | 18.684 | 12.964 | 1.00 | 21.83 |
| 5074 | O | THR | B | 56 | 8.671 | 19.001 | 11.808 | 1.00 | 21.23 |
| 5075 | N | MET | B | 57 | 9.220 | 17.953 | 13.728 | 1.00 | 21.95 |
| 5077 | CA | MET | B | 57 | 10.470 | 17.408 | 13.215 | 1.00 | 21.91 |
| 5079 | CB | MET | B | 57 | 11.207 | 16.630 | 14.299 | 1.00 | 21.87 |
| 5082 | CG | MET | B | 57 | 11.735 | 17.485 | 15.441 | 1.00 | 20.93 |
| 5085 | SD | MET | B | 57 | 12.315 | 16.444 | 16.774 | 1.00 | 22.35 |
| 5086 | CE | MET | B | 57 | 13.754 | 15.689 | 16.047 | 1.00 | 23.07 |
| 5090 | C | MET | B | 57 | 10.221 | 16.502 | 12.014 | 1.00 | 22.56 |
| 5091 | O | MET | B | 57 | 10.951 | 16.565 | 11.024 | 1.00 | 22.83 |
| 5092 | N | GLN | B | 58 | 9.179 | 15.676 | 12.088 | 1.00 | 23.09 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 5094 | CA | GLN | B | 58 | 8.895 | 14.714 | 11.016 | 1.00 | 23.09 |
| 5096 | CB | GLN | B | 58 | 7.843 | 13.694 | 11.460 | 1.00 | 23.18 |
| 5099 | CG | GLN | B | 58 | 8.386 | 12.700 | 12.456 | 1.00 | 24.11 |
| 5102 | CD | GLN | B | 58 | 7.334 | 11.743 | 12.961 | 1.00 | 26.66 |
| 5103 | OE1 | GLN | B | 58 | 7.463 | 10.525 | 12.791 | 1.00 | 28.62 |
| 5104 | NE2 | GLN | B | 58 | 6.304 | 12.280 | 13.601 | 1.00 | 23.91 |
| 5107 | C | GLN | B | 58 | 8.393 | 15.435 | 9.787 | 1.00 | 22.65 |
| 5108 | O | GLN | B | 58 | 8.764 | 15.123 | 8.661 | 1.00 | 22.15 |
| 5109 | N | TYR | B | 59 | 7.531 | 16.402 | 10.028 | 1.00 | 22.64 |
| 5111 | CA | TYR | B | 59 | 6.942 | 17.213 | 8.974 | 1.00 | 22.81 |
| 5113 | CB | TYR | B | 59 | 5.939 | 18.145 | 9.647 | 1.00 | 23.23 |
| 5116 | CG | TYR | B | 59 | 5.133 | 19.066 | 8.784 | 1.00 | 24.77 |
| 5117 | CD1 | TYR | B | 59 | 3.855 | 18.706 | 8.346 | 1.00 | 27.29 |
| 5119 | CE1 | TYR | B | 59 | 3.089 | 19.572 | 7.587 | 1.00 | 28.69 |
| 5121 | CZ | TYR | B | 59 | 3.582 | 20.820 | 7.286 | 1.00 | 28.49 |
| 5122 | OH | TYR | B | 59 | 2.827 | 21.673 | 6.537 | 1.00 | 28.74 |
| 5124 | CE2 | TYR | B | 59 | 4.844 | 21.209 | 7.727 | 1.00 | 27.93 |
| 5126 | CD2 | TYR | B | 59 | 5.600 | 20.335 | 8.477 | 1.00 | 26.79 |
| 5128 | C | TYR | B | 59 | 8.051 | 17.978 | 8.237 | 1.00 | 22.85 |
| 5129 | O | TYR | B | 59 | 8.114 | 17.976 | 7.010 | 1.00 | 22.68 |
| 5130 | N | GLY | B | 60 | 8.948 | 18.591 | 9.005 | 1.00 | 22.75 |
| 5132 | CA | GLY | B | 60 | 10.014 | 19.408 | 8.455 | 1.00 | 22.25 |
| 5135 | C | GLY | B | 60 | 11.071 | 18.608 | 7.738 | 1.00 | 22.08 |
| 5136 | O | GLY | B | 60 | 11.669 | 19.088 | 6.782 | 1.00 | 21.36 |
| 5137 | N | ALA | B | 61 | 11.310 | 17.384 | 8.201 | 1.00 | 22.33 |
| 5139 | CA | ALA | B | 61 | 12.382 | 16.568 | 7.656 | 1.00 | 22.52 |
| 5141 | CB | ALA | B | 61 | 12.996 | 15.714 | 8.733 | 1.00 | 22.31 |
| 5145 | C | ALA | B | 61 | 11.925 | 15.698 | 6.492 | 1.00 | 23.07 |
| 5146 | O | ALA | B | 61 | 12.692 | 15.487 | 5.548 | 1.00 | 22.77 |
| 5147 | N | LEU | B | 62 | 10.682 | 15.220 | 6.538 | 1.00 | 23.33 |
| 5149 | CA | LEU | B | 62 | 10.265 | 14.079 | 5.705 | 1.00 | 24.30 |
| 5151 | CB | LEU | B | 62 | 9.706 | 12.960 | 6.586 | 1.00 | 24.12 |
| 5154 | CG | LEU | B | 62 | 10.789 | 12.220 | 7.367 | 1.00 | 24.95 |
| 5156 | CD1 | LEU | B | 62 | 10.177 | 11.362 | 8.448 | 1.00 | 25.81 |
| 5160 | CD2 | LEU | B | 62 | 11.624 | 11.386 | 6.415 | 1.00 | 25.72 |
| 5164 | C | LEU | B | 62 | 9.241 | 14.390 | 4.610 | 1.00 | 24.83 |
| 5165 | O | LEU | B | 62 | 9.168 | 13.668 | 3.615 | 1.00 | 24.82 |
| 5166 | N | LEU | B | 63 | 8.480 | 15.459 | 4.784 | 1.00 | 25.44 |
| 5168 | CA | LEU | B | 63 | 7.363 | 15.761 | 3.890 | 1.00 | 26.38 |
| 5170 | CB | LEU | B | 63 | 6.196 | 16.353 | 4.683 | 1.00 | 26.51 |
| 5173 | CG | LEU | B | 63 | 4.851 | 15.625 | 4.607 | 1.00 | 29.53 |
| 5175 | CD1 | LEU | B | 63 | 4.953 | 14.108 | 4.807 | 1.00 | 30.58 |
| 5179 | CD2 | LEU | B | 63 | 3.880 | 16.228 | 5.625 | 1.00 | 30.77 |
| 5183 | C | LEU | B | 63 | 7.833 | 16.671 | 2.741 | 1.00 | 26.06 |
| 5184 | O | LEU | B | 63 | 7.862 | 17.895 | 2.846 | 1.00 | 27.01 |
| 5185 | N | GLY | B | 64 | 8.237 | 16.048 | 1.651 | 1.00 | 25.60 |
| 5187 | CA | GLY | B | 64 | 8.677 | 16.778 | 0.477 | 1.00 | 25.47 |
| 5190 | C | GLY | B | 64 | 10.152 | 17.095 | 0.529 | 1.00 | 24.67 |
| 5191 | O | GLY | B | 64 | 10.821 | 16.878 | 1.542 | 1.00 | 24.85 |
| 5192 | N | GLY | B | 65 | 10.655 | 17.628 | -0.575 | 1.00 | 24.17 |
| 5194 | CA | GLY | B | 65 | 12.046 | 18.001 | -0.702 | 1.00 | 23.50 |
| 5197 | C | GLY | B | 65 | 12.688 | 17.037 | -1.671 | 1.00 | 23.34 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 5198 | O | GLY | B | 65 | 12.221 | 15.901 | -1.822 | 1.00 | 23.79 |
| 5199 | N | LYS | B | 66 | 13.776 | 17.465 | -2.305 | 1.00 | 22.25 |
| 5201 | CA | LYS | B | 66 | 14.378 | 16.698 | -3.397 | 1.00 | 21.47 |
| 5203 | CB | LYS | B | 66 | 14.964 | 17.634 | -4.446 | 1.00 | 21.33 |
| 5206 | CG | LYS | B | 66 | 13.989 | 18.633 | -5.009 | 1.00 | 21.64 |
| 5209 | CD | LYS | B | 66 | 14.690 | 19.563 | -5.983 | 1.00 | 20.05 |
| 5212 | CE | LYS | B | 66 | 15.503 | 20.635 | -5.285 | 1.00 | 20.61 |
| 5215 | NZ | LYS | B | 66 | 14.661 | 21.571 | -4.488 | 1.00 | 18.47 |
| 5219 | C | LYS | B | 66 | 15.473 | 15.764 | -2.916 | 1.00 | 20.81 |
| 5220 | O | LYS | B | 66 | 15.930 | 14.904 | -3.680 | 1.00 | 19.71 |
| 5221 | N | ARG | B | 67 | 15.873 | 15.934 | -1.651 | 1.00 | 19.67 |
| 5223 | CA | ARG | B | 67 | 16.956 | 15.168 | -1.037 | 1.00 | 19.66 |
| 5225 | CB | ARG | B | 67 | 16.531 | 13.713 | -0.785 | 1.00 | 19.62 |
| 5228 | CG | ARG | B | 67 | 15.280 | 13.581 | 0.031 | 1.00 | 20.32 |
| 5231 | CD | ARG | B | 67 | 15.456 | 13.814 | 1.534 | 1.00 | 21.36 |
| 5234 | NE | ARG | B | 67 | 14.145 | 13.667 | 2.159 | 1.00 | 22.35 |
| 5236 | CZ | ARG | B | 67 | 13.232 | 14.625 | 2.243 | 1.00 | 24.57 |
| 5237 | NH1 | ARG | B | 67 | 13.491 | 15.867 | 1.836 | 1.00 | 25.55 |
| 5240 | NH2 | ARG | B | 67 | 12.042 | 14.347 | 2.754 | 1.00 | 25.42 |
| 5243 | C | ARG | B | 67 | 18.218 | 15.188 | -1.878 | 1.00 | 19.19 |
| 5244 | O | ARG | B | 67 | 18.871 | 14.162 | -2.042 | 1.00 | 19.59 |
| 5245 | N | LEU | B | 68 | 18.575 | 16.345 | -2.419 | 1.00 | 18.57 |
| 5247 | CA | LEU | B | 68 | 19.781 | 16.421 | -3.233 | 1.00 | 18.09 |
| 5249 | CB | LEU | B | 68 | 19.801 | 17.700 | -4.043 | 1.00 | 18.16 |
| 5252 | CG | LEU | B | 68 | 18.659 | 17.854 | -5.069 | 1.00 | 17.75 |
| 5254 | CD1 | LEU | B | 68 | 18.918 | 19.010 | -5.960 | 1.00 | 17.68 |
| 5258 | CD2 | LEU | B | 68 | 18.460 | 16.582 | -5.902 | 1.00 | 17.92 |
| 5262 | C | LEU | B | 68 | 21.050 | 16.265 | -2.398 | 1.00 | 18.27 |
| 5263 | O | LEU | B | 68 | 22.075 | 15.828 | -2.904 | 1.00 | 19.36 |
| 5264 | N | ARG | B | 69 | 20.984 | 16.589 | -1.118 | 1.00 | 18.60 |
| 5266 | CA | ARG | B | 69 | 22.152 | 16.472 | -0.263 | 1.00 | 18.77 |
| 5268 | CB | ARG | B | 69 | 22.052 | 17.389 | 0.948 | 1.00 | 18.34 |
| 5271 | CG | ARG | B | 69 | 22.255 | 18.855 | 0.557 | 1.00 | 18.92 |
| 5274 | CD | ARG | B | 69 | 21.763 | 19.861 | 1.576 | 1.00 | 19.63 |
| 5277 | NE | ARG | B | 69 | 21.626 | 21.189 | 0.993 | 1.00 | 18.86 |
| 5279 | CZ | ARG | B | 69 | 20.623 | 21.574 | 0.213 | 1.00 | 20.23 |
| 5280 | NH1 | ARG | B | 69 | 20.591 | 22.816 | -0.258 | 1.00 | 20.75 |
| 5283 | NH2 | ARG | B | 69 | 19.642 | 20.736 | -0.106 | 1.00 | 20.23 |
| 5286 | C | ARG | B | 69 | 22.421 | 14.999 | 0.076 | 1.00 | 19.10 |
| 5287 | O | ARG | B | 69 | 23.547 | 14.561 | -0.077 | 1.00 | 19.88 |
| 5288 | N | PRO | B | 70 | 21.423 | 14.225 | 0.504 | 1.00 | 19.43 |
| 5289 | CA | PRO | B | 70 | 21.571 | 12.764 | 0.495 | 1.00 | 19.41 |
| 5291 | CB | PRO | B | 70 | 20.168 | 12.271 | 0.822 | 1.00 | 20.11 |
| 5294 | CG | PRO | B | 70 | 19.619 | 13.337 | 1.712 | 1.00 | 19.65 |
| 5297 | CD | PRO | B | 70 | 20.136 | 14.628 | 1.091 | 1.00 | 19.55 |
| 5300 | C | PRO | B | 70 | 22.061 | 12.230 | -0.851 | 1.00 | 18.78 |
| 5301 | O | PRO | B | 70 | 22.971 | 11.411 | -0.850 | 1.00 | 19.31 |
| 5302 | N | PHE | B | 71 | 21.512 | 12.708 | -1.965 | 1.00 | 18.78 |
| 5304 | CA | PHE | B | 71 | 21.994 | 12.301 | -3.290 | 1.00 | 18.13 |
| 5306 | CB | PHE | B | 71 | 21.301 | 13.089 | -4.406 | 1.00 | 18.17 |
| 5309 | CG | PHE | B | 71 | 21.440 | 12.462 | -5.768 | 1.00 | 19.67 |
| 5310 | CD1 | PHE | B | 71 | 22.618 | 12.595 | -6.496 | 1.00 | 21.70 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 5312 | CE1 | PHE | B | 71 | 22.745 | 12.007 | -7.755 | 1.00 | 22.62 |
| 5314 | CZ | PHE | B | 71 | 21.697 | 11.280 | -8.296 | 1.00 | 23.33 |
| 5316 | CE2 | PHE | B | 71 | 20.532 | 11.138 | -7.587 | 1.00 | 23.93 |
| 5318 | CD2 | PHE | B | 71 | 20.400 | 11.730 | -6.324 | 1.00 | 22.20 |
| 5320 | C | PHE | B | 71 | 23.518 | 12.444 | -3.401 | 1.00 | 18.01 |
| 5321 | O | PHE | B | 71 | 24.194 | 11.528 | -3.851 | 1.00 | 17.71 |
| 5322 | N | LEU | B | 72 | 24.042 | 13.591 | -2.986 | 1.00 | 17.36 |
| 5324 | CA | LEU | B | 72 | 25.470 | 13.851 | -3.011 | 1.00 | 17.79 |
| 5326 | CB | LEU | B | 72 | 25.775 | 15.297 | -2.615 | 1.00 | 17.54 |
| 5329 | CG | LEU | B | 72 | 25.431 | 16.355 | -3.650 | 1.00 | 18.09 |
| 5331 | CD1 | LEU | B | 72 | 25.477 | 17.733 | -3.004 | 1.00 | 20.27 |
| 5335 | CD2 | LEU | B | 72 | 26.378 | 16.312 | -4.830 | 1.00 | 18.85 |
| 5339 | C | LEU | B | 72 | 26.245 | 12.913 | -2.104 | 1.00 | 17.24 |
| 5340 | O | LEU | B | 72 | 27.325 | 12.470 | -2.464 | 1.00 | 17.66 |
| 5341 | N | VAL | B | 73 | 25.717 | 12.633 | -0.920 | 1.00 | 16.80 |
| 5343 | CA | VAL | B | 73 | 26.388 | 11.711 | -0.011 | 1.00 | 16.74 |
| 5345 | CB | VAL | B | 73 | 25.658 | 11.640 | 1.340 | 1.00 | 16.98 |
| 5347 | CG1 | VAL | B | 73 | 26.180 | 10.504 | 2.196 | 1.00 | 16.26 |
| 5351 | CG2 | VAL | B | 73 | 25.754 | 13.004 | 2.088 | 1.00 | 17.68 |
| 5355 | C | VAL | B | 73 | 26.465 | 10.322 | -0.656 | 1.00 | 16.74 |
| 5356 | O | VAL | B | 73 | 27.536 | 9.725 | -0.718 | 1.00 | 15.63 |
| 5357 | N | TYR | B | 74 | 25.315 | 9.830 | -1.120 | 1.00 | 17.27 |
| 5359 | CA | TYR | B | 74 | 25.226 | 8.520 | -1.767 | 1.00 | 18.14 |
| 5361 | CB | TYR | B | 74 | 23.790 | 8.181 | -2.162 | 1.00 | 18.15 |
| 5364 | CG | TYR | B | 74 | 22.884 | 7.903 | -1.001 | 1.00 | 17.89 |
| 5365 | CD1 | TYR | B | 74 | 23.205 | 6.940 | -0.059 | 1.00 | 19.51 |
| 5367 | CE1 | TYR | B | 74 | 22.357 | 6.678 | 1.022 | 1.00 | 18.10 |
| 5369 | CZ | TYR | B | 74 | 21.198 | 7.396 | 1.155 | 1.00 | 18.28 |
| 5370 | OH | TYR | B | 74 | 20.351 | 7.135 | 2.215 | 1.00 | 19.90 |
| 5372 | CE2 | TYR | B | 74 | 20.866 | 8.363 | 0.221 | 1.00 | 18.45 |
| 5374 | CD2 | TYR | B | 74 | 21.699 | 8.599 | -0.846 | 1.00 | 18.98 |
| 5376 | C | TYR | B | 74 | 26.082 | 8.438 | -3.015 | 1.00 | 17.83 |
| 5377 | O | TYR | B | 74 | 26.788 | 7.478 | -3.201 | 1.00 | 17.93 |
| 5378 | N | ALA | B | 75 | 26.031 | 9.456 | -3.868 | 1.00 | 18.14 |
| 5380 | CA | ALA | B | 75 | 26.687 | 9.377 | -5.168 | 1.00 | 17.87 |
| 5382 | CB | ALA | B | 75 | 26.264 | 10.525 | -6.039 | 1.00 | 18.36 |
| 5386 | C | ALA | B | 75 | 28.200 | 9.387 | -4.975 | 1.00 | 18.40 |
| 5387 | O | ALA | B | 75 | 28.960 | 8.703 | -5.696 | 1.00 | 18.10 |
| 5388 | N | THR | B | 76 | 28.639 | 10.155 | -3.985 | 1.00 | 18.02 |
| 5390 | CA | THR | B | 76 | 30.055 | 10.258 | -3.691 | 1.00 | 18.66 |
| 5392 | CB | THR | B | 76 | 30.300 | 11.424 | -2.750 | 1.00 | 17.72 |
| 5394 | OG1 | THR | B | 76 | 29.858 | 12.636 | -3.373 | 1.00 | 18.73 |
| 5396 | CG2 | THR | B | 76 | 31.801 | 11.638 | -2.534 | 1.00 | 19.07 |
| 5400 | C | THR | B | 76 | 30.634 | 8.968 | -3.097 | 1.00 | 19.24 |
| 5401 | O | THR | B | 76 | 31.644 | 8.449 | -3.592 | 1.00 | 19.75 |
| 5402 | N | GLY | B | 77 | 29.999 | 8.474 | -2.036 | 1.00 | 19.50 |
| 5404 | CA | GLY | B | 77 | 30.432 | 7.259 | -1.389 | 1.00 | 20.08 |
| 5407 | C | GLY | B | 77 | 30.417 | 6.071 | -2.343 | 1.00 | 20.27 |
| 5408 | O | GLY | B | 77 | 31.314 | 5.231 | -2.310 | 1.00 | 20.87 |
| 5409 | N | HIS | B | 78 | 29.379 | 6.008 | -3.169 | 1.00 | 20.75 |
| 5411 | CA | HIS | B | 78 | 29.201 | 4.952 | -4.163 | 1.00 | 21.28 |
| 5413 | CB | HIS | B | 78 | 27.909 | 5.167 | -4.955 | 1.00 | 20.79 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 5416 | CG | HIS | B | 78 | 26.666 | 4.749 | -4.233 | 1.00 | 20.15 |
| 5417 | ND1 | HIS | B | 78 | 25.407 | 4.975 | -4.744 | 1.00 | 18.98 |
| 5419 | CE1 | HIS | B | 78 | 24.500 | 4.502 | -3.911 | 1.00 | 20.13 |
| 5421 | NE2 | HIS | B | 78 | 25.126 | 3.949 | -2.887 | 1.00 | 20.74 |
| 5423 | CD2 | HIS | B | 78 | 26.482 | 4.101 | -3.059 | 1.00 | 21.64 |
| 5425 | C | HIS | B | 78 | 30.361 | 4.878 | -5.151 | 1.00 | 21.89 |
| 5426 | O | HIS | B | 78 | 30.692 | 3.791 | -5.606 | 1.00 | 21.76 |
| 5427 | N | MET | B | 79 | 30.960 | 6.023 | -5.493 | 1.00 | 22.15 |
| 5429 | CA | MET | B | 79 | 32.157 | 6.051 | -6.357 | 1.00 | 23.42 |
| 5431 | CB | MET | B | 79 | 32.672 | 7.481 | -6.565 | 1.00 | 23.57 |
| 5434 | CG | MET | B | 79 | 31.804 | 8.325 | -7.471 | 1.00 | 24.99 |
| 5437 | SD | MET | B | 79 | 32.611 | 9.844 | -8.067 | 1.00 | 26.07 |
| 5438 | CE | MET | B | 79 | 33.270 | 10.463 | -6.588 | 1.00 | 25.93 |
| 5442 | C | MET | B | 79 | 33.303 | 5.200 | -5.819 | 1.00 | 23.68 |
| 5443 | O | MET | B | 79 | 34.094 | 4.657 | -6.595 | 1.00 | 24.77 |
| 5444 | N | PHE | B | 80 | 33.405 | 5.105 | -4.502 | 1.00 | 23.69 |
| 5446 | CA | PHE | B | 80 | 34.474 | 4.342 | -3.856 | 1.00 | 23.70 |
| 5448 | CB | PHE | B | 80 | 35.073 | 5.171 | -2.720 | 1.00 | 23.12 |
| 5451 | CG | PHE | B | 80 | 35.419 | 6.571 | -3.134 | 1.00 | 23.22 |
| 5452 | CD1 | PHE | B | 80 | 34.539 | 7.620 | -2.887 | 1.00 | 22.52 |
| 5454 | CE1 | PHE | B | 80 | 34.842 | 8.909 | -3.297 | 1.00 | 21.95 |
| 5456 | CZ | PHE | B | 80 | 36.029 | 9.160 | -3.967 | 1.00 | 23.61 |
| 5458 | CE2 | PHE | B | 80 | 36.910 | 8.116 | -4.230 | 1.00 | 22.42 |
| 5460 | CD2 | PHE | B | 80 | 36.604 | 6.834 | -3.818 | 1.00 | 23.20 |
| 5462 | C | PHE | B | 80 | 34.016 | 2.986 | -3.339 | 1.00 | 23.73 |
| 5463 | O | PHE | B | 80 | 34.751 | 2.309 | -2.625 | 1.00 | 23.67 |
| 5464 | N | GLY | B | 81 | 32.791 | 2.607 | -3.686 | 1.00 | 23.96 |
| 5466 | CA | GLY | B | 81 | 32.273 | 1.287 | -3.397 | 1.00 | 24.04 |
| 5469 | C | GLY | B | 81 | 31.674 | 1.153 | -2.023 | 1.00 | 23.99 |
| 5470 | O | GLY | B | 81 | 31.462 | 0.038 | -1.543 | 1.00 | 23.68 |
| 5471 | N | VAL | B | 82 | 31.385 | 2.278 | -1.375 | 1.00 | 23.71 |
| 5473 | CA | VAL | B | 82 | 30.866 | 2.207 | -0.020 | 1.00 | 23.08 |
| 5475 | CB | BVAL | B | 82 | 31.048 | 3.547 | 0.736 | 0.35 | 22.92 |
| 5476 | CB | AVAL | B | 82 | 31.192 | 3.459 | 0.840 | 0.65 | 23.42 |
| 5479 | CG1 | BVAL | B | 82 | 30.368 | 3.508 | 2.114 | 0.35 | 22.09 |
| 5480 | CG1 | AVAL | B | 82 | 32.625 | 3.934 | 0.590 | 0.65 | 23.81 |
| 5487 | CG2 | BVAL | B | 82 | 32.527 | 3.883 | 0.872 | 0.35 | 23.15 |
| 5488 | CG2 | AVAL | B | 82 | 30.219 | 4.544 | 0.625 | 0.65 | 24.67 |
| 5495 | C | VAL | B | 82 | 29.387 | 1.847 | -0.088 | 1.00 | 22.55 |
| 5496 | O | VAL | B | 82 | 28.660 | 2.300 | -0.965 | 1.00 | 21.42 |
| 5497 | N | SER | B | 83 | 28.987 | 0.968 | 0.819 | 1.00 | 22.22 |
| 5499 | CA | SER | B | 83 | 27.645 | 0.429 | 0.868 | 1.00 | 22.25 |
| 5501 | CB | SER | B | 83 | 27.539 | -0.621 | 1.979 | 1.00 | 22.22 |
| 5504 | OG | SER | B | 83 | 26.202 | -1.078 | 2.137 | 1.00 | 22.42 |
| 5506 | C | SER | B | 83 | 26.656 | 1.550 | 1.108 | 1.00 | 22.33 |
| 5507 | O | SER | B | 83 | 26.919 | 2.462 | 1.898 | 1.00 | 21.77 |
| 5508 | N | THR | B | 84 | 25.534 | 1.480 | 0.394 | 1.00 | 21.99 |
| 5510 | CA | THR | B | 84 | 24.431 | 2.400 | 0.559 | 1.00 | 22.06 |
| 5512 | CB | THR | B | 84 | 23.259 | 1.990 | -0.367 | 1.00 | 22.16 |
| 5514 | OG1 | THR | B | 84 | 23.685 | 2.032 | -1.732 | 1.00 | 23.21 |
| 5516 | CG2 | THR | B | 84 | 22.126 | 2.999 | -0.303 | 1.00 | 22.58 |
| 5520 | C | THR | B | 84 | 23.949 | 2.433 | 1.997 | 1.00 | 21.59 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 5521 | O | THR | B | 84 | 23.618 | 3.500 | 2.527 | 1.00 | 21.04 |
| 5522 | N | ASN | B | 85 | 23.897 | 1.261 | 2.628 | 1.00 | 21.29 |
| 5524 | CA | ASN | B | 85 | 23.467 | 1.170 | 4.022 | 1.00 | 21.08 |
| 5526 | CB | ASN | B | 85 | 23.358 | -0.293 | 4.454 | 1.00 | 21.68 |
| 5529 | CG | ASN | B | 85 | 23.046 | -0.442 | 5.923 | 1.00 | 21.92 |
| 5530 | OD1 | ASN | B | 85 | 21.903 | -0.297 | 6.343 | 1.00 | 23.33 |
| 5531 | ND2 | ASN | B | 85 | 24.060 | -0.747 | 6.706 | 1.00 | 22.60 |
| 5534 | C | ASN | B | 85 | 24.404 | 1.930 | 4.963 | 1.00 | 20.60 |
| 5535 | O | ASN | B | 85 | 23.950 | 2.532 | 5.920 | 1.00 | 19.95 |
| 5536 | N | THR | B | 86 | 25.708 | 1.876 | 4.708 | 1.00 | 20.20 |
| 5538 | CA | THR | B | 86 | 26.661 | 2.698 | 5.453 | 1.00 | 20.29 |
| 5540 | CB | THR | B | 86 | 28.086 | 2.339 | 5.017 | 1.00 | 20.31 |
| 5542 | OG1 | THR | B | 86 | 28.386 | 1.014 | 5.482 | 1.00 | 20.98 |
| 5544 | CG2 | THR | B | 86 | 29.139 | 3.242 | 5.699 | 1.00 | 21.55 |
| 5548 | C | THR | B | 86 | 26.390 | 4.199 | 5.257 | 1.00 | 20.17 |
| 5549 | O | THR | B | 86 | 26.440 | 4.994 | 6.218 | 1.00 | 20.64 |
| 5550 | N | LEU | B | 87 | 26.078 | 4.560 | 4.013 | 1.00 | 19.46 |
| 5552 | CA | LEU | B | 87 | 25.883 | 5.947 | 3.604 | 1.00 | 19.22 |
| 5554 | CB | LEU | B | 87 | 25.952 | 6.044 | 2.077 | 1.00 | 18.97 |
| 5557 | CG | LEU | B | 87 | 27.376 | 5.905 | 1.533 | 1.00 | 19.26 |
| 5559 | CD1 | LEU | B | 87 | 27.370 | 5.638 | 0.037 | 1.00 | 20.15 |
| 5563 | CD2 | LEU | B | 87 | 28.251 | 7.121 | 1.875 | 1.00 | 20.46 |
| 5567 | C | LEU | B | 87 | 24.584 | 6.574 | 4.113 | 1.00 | 19.19 |
| 5568 | O | LEU | B | 87 | 24.445 | 7.794 | 4.139 | 1.00 | 18.91 |
| 5569 | N | ASP | B | 88 | 23.641 | 5.746 | 4.523 | 1.00 | 19.51 |
| 5571 | CA | ASP | B | 88 | 22.393 | 6.219 | 5.106 | 1.00 | 19.28 |
| 5573 | CB | ASP | B | 88 | 21.559 | 5.046 | 5.616 | 1.00 | 19.89 |
| 5576 | CG | ASP | B | 88 | 20.654 | 4.406 | 4.552 | 1.00 | 21.00 |
| 5577 | OD1 | ASP | B | 88 | 20.591 | 4.823 | 3.365 | 1.00 | 21.03 |
| 5578 | OD2 | ASP | B | 88 | 19.938 | 3.431 | 4.867 | 1.00 | 24.24 |
| 5579 | C | ASP | B | 88 | 22.645 | 7.167 | 6.297 | 1.00 | 18.72 |
| 5580 | O | ASP | B | 88 | 21.924 | 8.147 | 6.462 | 1.00 | 18.18 |
| 5581 | N | ALA | B | 89 | 23.639 | 6.861 | 7.130 | 1.00 | 18.70 |
| 5583 | CA | ALA | B | 89 | 23.955 | 7.700 | 8.290 | 1.00 | 19.48 |
| 5585 | CB | ALA | B | 89 | 25.006 | 7.061 | 9.204 | 1.00 | 19.64 |
| 5589 | C | ALA | B | 89 | 24.360 | 9.113 | 7.894 | 1.00 | 19.16 |
| 5590 | O | ALA | B | 89 | 23.679 | 10.049 | 8.257 | 1.00 | 18.92 |
| 5591 | N | PRO | B | 90 | 25.451 | 9.305 | 7.163 | 1.00 | 19.56 |
| 5592 | CA | PRO | B | 90 | 25.781 | 10.672 | 6.739 | 1.00 | 19.16 |
| 5594 | CB | PRO | B | 90 | 27.114 | 10.519 | 6.004 | 1.00 | 19.21 |
| 5597 | CG | PRO | B | 90 | 27.166 | 9.070 | 5.606 | 1.00 | 19.67 |
| 5600 | CD | PRO | B | 90 | 26.446 | 8.323 | 6.694 | 1.00 | 19.64 |
| 5603 | C | PRO | B | 90 | 24.692 | 11.299 | 5.856 | 1.00 | 18.58 |
| 5604 | O | PRO | B | 90 | 24.509 | 12.510 | 5.924 | 1.00 | 18.13 |
| 5605 | N | ALA | B | 91 | 23.975 | 10.506 | 5.063 | 1.00 | 18.37 |
| 5607 | CA | ALA | B | 91 | 22.891 | 11.038 | 4.225 | 1.00 | 18.51 |
| 5609 | CB | ALA | B | 91 | 22.314 | 9.952 | 3.312 | 1.00 | 18.83 |
| 5613 | C | ALA | B | 91 | 21.790 | 11.644 | 5.073 | 1.00 | 18.64 |
| 5614 | O | ALA | B | 91 | 21.313 | 12.749 | 4.811 | 1.00 | 19.06 |
| 5615 | N | ALA | B | 92 | 21.407 | 10.928 | 6.114 | 1.00 | 18.40 |
| 5617 | CA | ALA | B | 92 | 20.360 | 11.383 | 7.010 | 1.00 | 18.11 |
| 5619 | CB | ALA | B | 92 | 19.906 | 10.245 | 7.903 | 1.00 | 18.05 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 5623 | C | ALA | B | 92 | 20.855 | 12.566 | 7.841 | 1.00 | 17.48 |
| 5624 | O | ALA | B | 92 | 20.123 | 13.505 | 8.071 | 1.00 | 16.95 |
| 5625 | N | ALA | B | 93 | 22.105 | 12.525 | 8.281 | 1.00 | 17.41 |
| 5627 | CA | ALA | B | 93 | 22.630 | 13.600 | 9.115 | 1.00 | 17.40 |
| 5629 | CB | ALA | B | 93 | 23.982 | 13.244 | 9.638 | 1.00 | 17.13 |
| 5633 | C | ALA | B | 93 | 22.680 | 14.917 | 8.335 | 1.00 | 17.61 |
| 5634 | O | ALA | B | 93 | 22.298 | 15.947 | 8.858 | 1.00 | 17.33 |
| 5635 | N | VAL | B | 94 | 23.143 | 14.893 | 7.091 | 1.00 | 18.42 |
| 5637 | CA | VAL | B | 94 | 23.208 | 16.146 | 6.304 | 1.00 | 18.96 |
| 5639 | CB | BVAL | B | 94 | 24.038 | 16.002 | 4.993 | 0.35 | 18.97 |
| 5640 | CB | AVAL | B | 94 | 23.983 | 16.016 | 4.957 | 0.65 | 19.14 |
| 5643 | CG1 | BVAL | B | 94 | 23.256 | 15.295 | 3.906 | 0.35 | 19.73 |
| 5644 | CG1 | AVAL | B | 94 | 25.429 | 15.726 | 5.214 | 0.65 | 19.11 |
| 5651 | CG2 | BVAL | B | 94 | 24.517 | 17.378 | 4.509 | 0.35 | 18.57 |
| 5652 | CG2 | AVAL | B | 94 | 23.381 | 14.977 | 4.031 | 0.65 | 20.34 |
| 5659 | C | VAL | B | 94 | 21.813 | 16.685 | 6.031 | 1.00 | 19.05 |
| 5660 | O | VAL | B | 94 | 21.610 | 17.902 | 6.048 | 1.00 | 19.83 |
| 5661 | N | GLU | B | 95 | 20.858 | 15.786 | 5.828 | 1.00 | 18.96 |
| 5663 | CA | GLU | B | 95 | 19.479 | 16.181 | 5.611 | 1.00 | 19.29 |
| 5665 | CB | GLU | B | 95 | 18.657 | 15.024 | 5.045 | 1.00 | 19.83 |
| 5668 | CG | GLU | B | 95 | 17.271 | 15.429 | 4.550 | 1.00 | 20.18 |
| 5671 | CD | GLU | B | 95 | 17.276 | 16.380 | 3.353 | 1.00 | 21.04 |
| 5672 | OE1 | GLU | B | 95 | 16.175 | 16.831 | 2.956 | 1.00 | 20.80 |
| 5673 | OE2 | GLU | B | 95 | 18.352 | 16.669 | 2.784 | 1.00 | 22.55 |
| 5674 | C | GLU | B | 95 | 18.816 | 16.727 | 6.868 | 1.00 | 19.09 |
| 5675 | O | GLU | B | 95 | 17.964 | 17.587 | 6.761 | 1.00 | 18.76 |
| 5676 | N | CYS | B | 96 | 19.205 | 16.246 | 8.053 | 1.00 | 19.19 |
| 5678 | CA | CYS | B | 96 | 18.694 | 16.808 | 9.313 | 1.00 | 18.68 |
| 5680 | CB | CYS | B | 96 | 19.186 | 16.019 | 10.519 | 1.00 | 19.12 |
| 5683 | SG | CYS | B | 96 | 18.326 | 14.474 | 10.771 | 1.00 | 22.59 |
| 5684 | C | CYS | B | 96 | 19.160 | 18.255 | 9.485 | 1.00 | 17.90 |
| 5685 | O | CYS | B | 96 | 18.407 | 19.095 | 9.978 | 1.00 | 17.58 |
| 5686 | N | ILE | B | 97 | 20.416 | 18.524 | 9.129 | 1.00 | 16.55 |
| 5688 | CA | ILE | B | 97 | 20.951 | 19.877 | 9.214 | 1.00 | 16.20 |
| 5690 | CB | ILE | B | 97 | 22.468 | 19.934 | 8.896 | 1.00 | 15.98 |
| 5692 | CG1 | ILE | B | 97 | 23.261 | 19.204 | 9.970 | 1.00 | 15.40 |
| 5695 | CD1 | ILE | B | 97 | 23.203 | 19.886 | 11.342 | 1.00 | 17.23 |
| 5699 | CG2 | ILE | B | 97 | 22.941 | 21.391 | 8.777 | 1.00 | 15.29 |
| 5703 | C | ILE | B | 97 | 20.200 | 20.722 | 8.215 | 1.00 | 15.87 |
| 5704 | O | ILE | B | 97 | 19.770 | 21.815 | 8.533 | 1.00 | 15.70 |
| 5705 | N | HIS | B | 98 | 20.067 | 20.215 | 6.992 | 1.00 | 15.91 |
| 5707 | CA | HIS | B | 98 | 19.330 | 20.914 | 5.957 | 1.00 | 16.10 |
| 5709 | CB | HIS | B | 98 | 19.247 | 20.072 | 4.687 | 1.00 | 16.66 |
| 5712 | CG | HIS | B | 98 | 18.572 | 20.782 | 3.567 | 1.00 | 15.86 |
| 5713 | ND1 | HIS | B | 98 | 17.518 | 20.240 | 2.860 | 1.00 | 19.53 |
| 5715 | CE1 | HIS | B | 98 | 17.127 | 21.104 | 1.941 | 1.00 | 17.62 |
| 5717 | NE2 | HIS | B | 98 | 17.871 | 22.190 | 2.043 | 1.00 | 19.93 |
| 5719 | CD2 | HIS | B | 98 | 18.776 | 22.017 | 3.057 | 1.00 | 15.34 |
| 5721 | C | HIS | B | 98 | 17.923 | 21.259 | 6.424 | 1.00 | 17.04 |
| 5722 | O | HIS | B | 98 | 17.524 | 22.425 | 6.412 | 1.00 | 16.67 |
| 5723 | N | ALA | B | 99 | 17.193 | 20.243 | 6.885 | 1.00 | 17.19 |
| 5725 | CA | ALA | B | 99 | 15.809 | 20.414 | 7.334 | 1.00 | 17.14 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 5727 | CB | ALA | B | 99 | 15.236 | 19.074 | 7.793 | 1.00 | 17.69 |
| 5731 | C | ALA | B | 99 | 15.681 | 21.456 | 8.452 | 1.00 | 17.97 |
| 5732 | O | ALA | B | 99 | 14.806 | 22.325 | 8.400 | 1.00 | 17.24 |
| 5733 | N | TYR | B | 100 | 16.570 | 21.389 | 9.449 | 1.00 | 17.80 |
| 5735 | CA | TYR | B | 100 | 16.550 | 22.348 | 10.560 | 1.00 | 17.32 |
| 5737 | CB | TYR | B | 100 | 17.580 | 21.968 | 11.647 | 1.00 | 18.17 |
| 5740 | CG | TYR | B | 100 | 18.635 | 23.015 | 11.933 | 1.00 | 19.38 |
| 5741 | CD1 | TYR | B | 100 | 18.308 | 24.219 | 12.556 | 1.00 | 22.96 |
| 5743 | CE1 | TYR | B | 100 | 19.290 | 25.186 | 12.809 | 1.00 | 23.47 |
| 5745 | CZ | TYR | B | 100 | 20.601 | 24.932 | 12.424 | 1.00 | 23.58 |
| 5746 | OH | TYR | B | 100 | 21.596 | 25.839 | 12.653 | 1.00 | 22.83 |
| 5748 | CE2 | TYR | B | 100 | 20.935 | 23.736 | 11.815 | 1.00 | 21.94 |
| 5750 | CD2 | TYR | B | 100 | 19.963 | 22.802 | 11.571 | 1.00 | 20.83 |
| 5752 | C | TYR | B | 100 | 16.810 | 23.765 | 10.042 | 1.00 | 16.90 |
| 5753 | O | TYR | B | 100 | 16.187 | 24.727 | 10.489 | 1.00 | 16.75 |
| 5754 | N | SER | B | 101 | 17.730 | 23.891 | 9.098 | 1.00 | 16.44 |
| 5756 | CA | SER | B | 101 | 18.097 | 25.192 | 8.581 | 1.00 | 17.14 |
| 5758 | CB | SER | B | 101 | 19.263 | 25.083 | 7.593 | 1.00 | 16.73 |
| 5761 | OG | SER | B | 101 | 18.840 | 24.597 | 6.337 | 1.00 | 18.73 |
| 5763 | C | SER | B | 101 | 16.887 | 25.851 | 7.924 | 1.00 | 17.47 |
| 5764 | O | SER | B | 101 | 16.686 | 27.050 | 8.047 | 1.00 | 17.44 |
| 5765 | N | LEU | B | 102 | 16.089 | 25.064 | 7.224 | 1.00 | 18.06 |
| 5767 | CA | LEU | B | 102 | 14.897 | 25.584 | 6.562 | 1.00 | 18.72 |
| 5769 | CB | LEU | B | 102 | 14.324 | 24.528 | 5.642 | 1.00 | 19.20 |
| 5772 | CG | LEU | B | 102 | 15.224 | 23.982 | 4.548 | 1.00 | 19.55 |
| 5774 | CD1 | LEU | B | 102 | 14.392 | 23.084 | 3.642 | 1.00 | 21.29 |
| 5778 | CD2 | LEU | B | 102 | 15.912 | 25.114 | 3.771 | 1.00 | 19.66 |
| 5782 | C | LEU | B | 102 | 13.814 | 26.018 | 7.551 | 1.00 | 18.78 |
| 5783 | O | LEU | B | 102 | 13.179 | 27.057 | 7.360 | 1.00 | 19.38 |
| 5784 | N | ILE | B | 103 | 13.607 | 25.227 | 8.599 | 1.00 | 18.35 |
| 5786 | CA | ILE | B | 103 | 12.581 | 25.536 | 9.612 | 1.00 | 18.39 |
| 5788 | CB | ILE | B | 103 | 12.525 | 24.456 | 10.724 | 1.00 | 18.49 |
| 5790 | CG1 | ILE | B | 103 | 12.050 | 23.122 | 10.161 | 1.00 | 19.38 |
| 5793 | CD1 | ILE | B | 103 | 12.339 | 21.950 | 11.075 | 1.00 | 20.40 |
| 5797 | CG2 | ILE | B | 103 | 11.617 | 24.887 | 11.862 | 1.00 | 18.22 |
| 5801 | C | ILE | B | 103 | 12.874 | 26.891 | 10.247 | 1.00 | 18.35 |
| 5802 | O | ILE | B | 103 | 11.976 | 27.698 | 10.437 | 1.00 | 18.38 |
| 5803 | N | HIS | B | 104 | 14.142 | 27.127 | 10.568 | 1.00 | 18.85 |
| 5805 | CA | HIS | B | 104 | 14.554 | 28.377 | 11.204 | 1.00 | 18.52 |
| 5807 | CB | HIS | B | 104 | 15.891 | 28.199 | 11.898 | 1.00 | 19.08 |
| 5810 | CG | HIS | B | 104 | 15.787 | 27.494 | 13.204 | 1.00 | 18.65 |
| 5811 | ND1 | HIS | B | 104 | 16.798 | 27.505 | 14.135 | 1.00 | 19.24 |
| 5813 | CE1 | HIS | B | 104 | 16.422 | 26.803 | 15.188 | 1.00 | 20.04 |
| 5815 | NE2 | HIS | B | 104 | 15.204 | 26.341 | 14.976 | 1.00 | 19.64 |
| 5817 | CD2 | HIS | B | 104 | 14.785 | 26.756 | 13.738 | 1.00 | 20.54 |
| 5819 | C | HIS | B | 104 | 14.588 | 29.526 | 10.189 | 1.00 | 18.70 |
| 5820 | O | HIS | B | 104 | 14.261 | 30.658 | 10.527 | 1.00 | 18.65 |
| 5821 | N | ASP | B | 105 | 14.949 | 29.218 | 8.946 | 1.00 | 18.55 |
| 5823 | CA | ASP | B | 105 | 14.971 | 30.199 | 7.861 | 1.00 | 18.61 |
| 5825 | CB | ASP | B | 105 | 15.515 | 29.530 | 6.605 | 1.00 | 18.44 |
| 5828 | CG | ASP | B | 105 | 15.629 | 30.470 | 5.456 | 1.00 | 18.37 |
| 5829 | OD1 | ASP | B | 105 | 14.710 | 30.462 | 4.590 | 1.00 | 16.28 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 5830 | OD2 | ASP | B | 105 | 16.618 | 31.233 | 5.324 | 1.00 | 20.63 |
| 5831 | C | ASP | B | 105 | 13.581 | 30.809 | 7.572 | 1.00 | 18.97 |
| 5832 | O | ASP | B | 105 | 13.471 | 31.985 | 7.256 | 1.00 | 19.10 |
| 5833 | N | ASP | B | 106 | 12.537 | 30.007 | 7.703 | 1.00 | 19.32 |
| 5835 | CA | ASP | B | 106 | 11.172 | 30.446 | 7.448 | 1.00 | 20.42 |
| 5837 | CB | ASP | B | 106 | 10.283 | 29.224 | 7.206 | 1.00 | 20.29 |
| 5840 | CG | ASP | B | 106 | 10.566 | 28.544 | 5.883 | 1.00 | 20.45 |
| 5841 | OD1 | ASP | B | 106 | 10.363 | 27.303 | 5.791 | 1.00 | 21.30 |
| 5842 | OD2 | ASP | B | 106 | 10.981 | 29.158 | 4.885 | 1.00 | 20.64 |
| 5843 | C | ASP | B | 106 | 10.524 | 31.287 | 8.577 | 1.00 | 20.97 |
| 5844 | O | ASP | B | 106 | 9.465 | 31.874 | 8.372 | 1.00 | 21.34 |
| 5845 | N | LEU | B | 107 | 11.150 | 31.332 | 9.748 | 1.00 | 21.55 |
| 5847 | CA | LEU | B | 107 | 10.588 | 31.991 | 10.925 | 1.00 | 22.27 |
| 5849 | CB | LEU | B | 107 | 11.551 | 31.861 | 12.120 | 1.00 | 22.07 |
| 5852 | CG | LEU | B | 107 | 11.746 | 30.451 | 12.684 | 1.00 | 22.57 |
| 5854 | CD1 | LEU | B | 107 | 12.901 | 30.397 | 13.690 | 1.00 | 21.96 |
| 5858 | CD2 | LEU | B | 107 | 10.471 | 29.947 | 13.317 | 1.00 | 23.63 |
| 5862 | C | LEU | B | 107 | 10.313 | 33.470 | 10.646 | 1.00 | 22.59 |
| 5863 | O | LEU | B | 107 | 11.025 | 34.078 | 9.870 | 1.00 | 22.10 |
| 5864 | N | PRO | B | 108 | 9.262 | 34.035 | 11.242 | 1.00 | 23.34 |
| 5865 | CA | PRO | B | 108 | 8.959 | 35.467 | 11.096 | 1.00 | 23.88 |
| 5867 | CB | PRO | B | 108 | 7.886 | 35.698 | 12.152 | 1.00 | 23.65 |
| 5870 | CG | PRO | B | 108 | 7.151 | 34.422 | 12.154 | 1.00 | 24.22 |
| 5873 | CD | PRO | B | 108 | 8.225 | 33.347 | 12.024 | 1.00 | 23.27 |
| 5876 | C | PRO | B | 108 | 10.131 | 36.428 | 11.282 | 1.00 | 24.08 |
| 5877 | O | PRO | B | 108 | 10.211 | 37.387 | 10.523 | 1.00 | 24.64 |
| 5878 | N | ALA | B | 109 | 11.019 | 36.183 | 12.243 | 1.00 | 24.21 |
| 5880 | CA | ALA | B | 109 | 12.179 | 37.054 | 12.450 | 1.00 | 24.56 |
| 5882 | CB | ALA | B | 109 | 12.804 | 36.795 | 13.823 | 1.00 | 24.65 |
| 5886 | C | ALA | B | 109 | 13.235 | 36.885 | 11.364 | 1.00 | 24.37 |
| 5887 | O | ALA | B | 109 | 14.092 | 37.756 | 11.188 | 1.00 | 25.00 |
| 5888 | N | MET | B | 110 | 13.193 | 35.747 | 10.674 | 1.00 | 23.93 |
| 5890 | CA | MET | B | 110 | 14.111 | 35.445 | 9.578 | 1.00 | 24.35 |
| 5892 | CB | MET | B | 110 | 14.527 | 33.969 | 9.642 | 1.00 | 24.14 |
| 5895 | CG | MET | B | 110 | 15.317 | 33.629 | 10.912 | 1.00 | 26.61 |
| 5898 | SD | MET | B | 110 | 17.063 | 34.058 | 10.820 | 1.00 | 29.08 |
| 5899 | CE | MET | B | 110 | 17.584 | 33.058 | 9.452 | 1.00 | 29.15 |
| 5903 | C | MET | B | 110 | 13.463 | 35.845 | 8.237 | 1.00 | 23.69 |
| 5904 | O | MET | B | 110 | 13.310 | 37.040 | 7.995 | 1.00 | 23.79 |
| 5905 | N | ASP | B | 111 | 13.044 | 34.885 | 7.404 | 1.00 | 23.23 |
| 5907 | CA | ASP | B | 111 | 12.489 | 35.198 | 6.073 | 1.00 | 22.98 |
| 5909 | CB | ASP | B | 111 | 12.936 | 34.167 | 5.016 | 1.00 | 22.62 |
| 5912 | CG | ASP | B | 111 | 14.429 | 34.138 | 4.838 | 1.00 | 21.61 |
| 5913 | OD1 | ASP | B | 111 | 14.957 | 33.260 | 4.090 | 1.00 | 18.84 |
| 5914 | OD2 | ASP | B | 111 | 15.163 | 34.963 | 5.413 | 1.00 | 21.22 |
| 5915 | C | ASP | B | 111 | 10.967 | 35.289 | 6.067 | 1.00 | 23.49 |
| 5916 | O | ASP | B | 111 | 10.365 | 35.645 | 5.054 | 1.00 | 22.75 |
| 5917 | N | ASP | B | 112 | 10.348 | 34.950 | 7.185 | 1.00 | 23.98 |
| 5919 | CA | ASP | B | 112 | 8.907 | 35.099 | 7.339 | 1.00 | 25.41 |
| 5921 | CB | ASP | B | 112 | 8.567 | 36.597 | 7.503 | 1.00 | 25.60 |
| 5924 | CG | ASP | B | 112 | 7.203 | 36.817 | 8.103 | 1.00 | 27.51 |
| 5925 | OD1 | ASP | B | 112 | 6.682 | 37.941 | 7.973 | 1.00 | 29.77 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 5926 | OD2 | ASP | B | 112 | 6.583 | 35.930 | 8.728 | 1.00 | 28.05 |
| 5927 | C | ASP | B | 112 | 8.126 | 34.503 | 6.172 | 1.00 | 25.57 |
| 5928 | O | ASP | B | 112 | 7.385 | 35.206 | 5.498 | 1.00 | 25.87 |
| 5929 | N | ASP | B | 113 | 8.309 | 33.203 | 5.936 | 1.00 | 26.04 |
| 5931 | CA | ASP | B | 113 | 7.630 | 32.487 | 4.861 | 1.00 | 25.95 |
| 5933 | CB | ASP | B | 113 | 8.641 | 31.685 | 4.032 | 1.00 | 26.04 |
| 5936 | CG | ASP | B | 113 | 9.212 | 32.477 | 2.895 | 1.00 | 26.93 |
| 5937 | OD1 | ASP | B | 113 | 8.428 | 32.869 | 2.004 | 1.00 | 30.09 |
| 5938 | OD2 | ASP | B | 113 | 10.426 | 32.755 | 2.786 | 1.00 | 25.96 |
| 5939 | C | ASP | B | 113 | 6.573 | 31.549 | 5.403 | 1.00 | 26.02 |
| 5940 | O | ASP | B | 113 | 6.773 | 30.883 | 6.425 | 1.00 | 26.50 |
| 5941 | N | ASP | B | 114 | 5.443 | 31.487 | 4.703 | 1.00 | 25.79 |
| 5943 | CA | ASP | B | 114 | 4.331 | 30.628 | 5.107 | 1.00 | 25.53 |
| 5945 | CB | ASP | B | 114 | 3.012 | 31.404 | 5.131 | 1.00 | 25.80 |
| 5948 | CG | ASP | B | 114 | 2.611 | 31.970 | 3.766 | 1.00 | 28.04 |
| 5949 | OD1 | ASP | B | 114 | 1.460 | 32.426 | 3.651 | 1.00 | 30.10 |
| 5950 | OD2 | ASP | B | 114 | 3.356 | 32.024 | 2.762 | 1.00 | 28.90 |
| 5951 | C | ASP | B | 114 | 4.183 | 29.359 | 4.260 | 1.00 | 24.50 |
| 5952 | O | ASP | B | 114 | 3.362 | 28.516 | 4.588 | 1.00 | 23.73 |
| 5953 | N | LEU | B | 115 | 4.975 | 29.228 | 3.197 | 1.00 | 23.97 |
| 5955 | CA | LEU | B | 115 | 4.939 | 28.054 | 2.323 | 1.00 | 23.69 |
| 5957 | CB | LEU | B | 115 | 4.386 | 28.414 | 0.940 | 1.00 | 24.10 |
| 5960 | CG | LEU | B | 115 | 2.907 | 28.201 | 0.569 | 1.00 | 27.09 |
| 5962 | CD1 | LEU | B | 115 | 2.748 | 28.570 | -0.917 | 1.00 | 27.23 |
| 5966 | CD2 | LEU | B | 115 | 2.367 | 26.794 | 0.840 | 1.00 | 25.73 |
| 5970 | C | LEU | B | 115 | 6.329 | 27.462 | 2.103 | 1.00 | 22.98 |
| 5971 | O | LEU | B | 115 | 7.271 | 28.178 | 1.813 | 1.00 | 22.51 |
| 5972 | N | ARG | B | 116 | 6.426 | 26.146 | 2.208 | 1.00 | 22.68 |
| 5974 | CA | ARG | B | 116 | 7.609 | 25.422 | 1.776 | 1.00 | 22.37 |
| 5976 | CB | ARG | B | 116 | 8.662 | 25.359 | 2.878 | 1.00 | 22.08 |
| 5979 | CG | ARG | B | 116 | 9.916 | 24.624 | 2.441 | 1.00 | 21.74 |
| 5982 | CD | ARG | B | 116 | 11.021 | 24.622 | 3.487 | 1.00 | 19.15 |
| 5985 | NE | ARG | B | 116 | 11.586 | 25.949 | 3.737 | 1.00 | 17.98 |
| 5987 | CZ | ARG | B | 116 | 12.421 | 26.579 | 2.911 | 1.00 | 18.36 |
| 5988 | NH1 | ARG | B | 116 | 12.900 | 27.771 | 3.239 | 1.00 | 19.16 |
| 5991 | NH2 | ARG | B | 116 | 12.789 | 26.027 | 1.770 | 1.00 | 18.06 |
| 5994 | C | ARG | B | 116 | 7.210 | 24.022 | 1.382 | 1.00 | 22.36 |
| 5995 | O | ARG | B | 116 | 6.409 | 23.385 | 2.071 | 1.00 | 22.81 |
| 5996 | N | ARG | B | 117 | 7.789 | 23.549 | 0.283 | 1.00 | 22.18 |
| 5998 | CA | ARG | B | 117 | 7.542 | 22.212 | -0.244 | 1.00 | 22.54 |
| 6000 | CB | ARG | B | 117 | 8.143 | 21.147 | 0.679 | 1.00 | 22.32 |
| 6003 | CG | ARG | B | 117 | 9.662 | 21.147 | 0.734 | 1.00 | 21.77 |
| 6006 | CD | ARG | B | 117 | 10.202 | 20.545 | 2.021 | 1.00 | 21.80 |
| 6009 | NE | ARG | B | 117 | 11.633 | 20.275 | 1.973 | 1.00 | 20.78 |
| 6011 | CZ | ARG | B | 117 | 12.305 | 19.671 | 2.947 | 1.00 | 20.45 |
| 6012 | NH1 | ARG | B | 117 | 11.688 | 19.269 | 4.048 | 1.00 | 18.82 |
| 6015 | NH2 | ARG | B | 117 | 13.608 | 19.464 | 2.826 | 1.00 | 19.98 |
| 6018 | C | ARG | B | 117 | 6.042 | 21.973 | -0.465 | 1.00 | 23.08 |
| 6019 | O | ARG | B | 117 | 5.544 | 20.861 | -0.338 | 1.00 | 22.39 |
| 6020 | N | GLY | B | 118 | 5.335 | 23.042 | -0.807 | 1.00 | 23.92 |
| 6022 | CA | GLY | B | 118 | 3.921 | 22.975 | -1.135 | 1.00 | 24.69 |
| 6025 | C | GLY | B | 118 | 3.010 | 23.023 | 0.070 | 1.00 | 24.98 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 6026 | O | GLY | B | 118 | 1.808 | 22.978 | -0.089 | 1.00 | 25.54 |
| 6027 | N | LEU | B | 119 | 3.578 | 23.126 | 1.268 | 1.00 | 25.57 |
| 6029 | CA | LEU | B | 119 | 2.813 | 23.045 | 2.508 | 1.00 | 25.94 |
| 6031 | CB | LEU | B | 119 | 3.226 | 21.797 | 3.283 | 1.00 | 26.65 |
| 6034 | CG | LEU | B | 119 | 3.068 | 20.468 | 2.548 | 1.00 | 29.36 |
| 6036 | CD1 | LEU | B | 119 | 3.750 | 19.369 | 3.338 | 1.00 | 31.10 |
| 6040 | CD2 | LEU | B | 119 | 1.599 | 20.127 | 2.336 | 1.00 | 31.06 |
| 6044 | C | LEU | B | 119 | 3.043 | 24.272 | 3.388 | 1.00 | 25.32 |
| 6045 | O | LEU | B | 119 | 4.027 | 24.999 | 3.216 | 1.00 | 24.34 |
| 6046 | N | PRO | B | 120 | 2.153 | 24.497 | 4.355 | 1.00 | 25.34 |
| 6047 | CA | PRO | B | 120 | 2.425 | 25.500 | 5.383 | 1.00 | 24.92 |
| 6049 | CB | PRO | B | 120 | 1.261 | 25.331 | 6.348 | 1.00 | 25.42 |
| 6052 | CG | PRO | B | 120 | 0.165 | 24.734 | 5.503 | 1.00 | 25.33 |
| 6055 | CD | PRO | B | 120 | 0.862 | 23.812 | 4.575 | 1.00 | 25.09 |
| 6058 | C | PRO | B | 120 | 3.764 | 25.201 | 6.077 | 1.00 | 24.65 |
| 6059 | O | PRO | B | 120 | 4.051 | 24.057 | 6.403 | 1.00 | 24.29 |
| 6060 | N | THR | B | 121 | 4.583 | 26.222 | 6.259 | 1.00 | 24.42 |
| 6062 | CA | THR | B | 121 | 5.850 | 26.062 | 6.966 | 1.00 | 24.49 |
| 6064 | CB | THR | B | 121 | 6.635 | 27.364 | 6.990 | 1.00 | 24.32 |
| 6066 | OG1 | THR | B | 121 | 5.798 | 28.437 | 7.465 | 1.00 | 26.32 |
| 6068 | CG2 | THR | B | 121 | 7.058 | 27.773 | 5.573 | 1.00 | 24.50 |
| 6072 | C | THR | B | 121 | 5.607 | 25.577 | 8.387 | 1.00 | 24.50 |
| 6073 | O | THR | B | 121 | 4.512 | 25.721 | 8.944 | 1.00 | 23.20 |
| 6074 | N | CYS | B | 122 | 6.641 | 24.995 | 8.969 | 1.00 | 24.26 |
| 6076 | CA | CYS | B | 122 | 6.537 | 24.419 | 10.297 | 1.00 | 24.93 |
| 6078 | CB | CYS | B | 122 | 7.885 | 23.869 | 10.759 | 1.00 | 24.70 |
| 6081 | SG | CYS | B | 122 | 8.346 | 22.384 | 9.881 | 1.00 | 26.74 |
| 6082 | C | CYS | B | 122 | 6.002 | 25.412 | 11.305 | 1.00 | 24.67 |
| 6083 | O | CYS | B | 122 | 5.204 | 25.042 | 12.148 | 1.00 | 25.48 |
| 6084 | N | HIS | B | 123 | 6.408 | 26.672 | 11.212 | 1.00 | 24.78 |
| 6086 | CA | HIS | B | 123 | 5.981 | 27.647 | 12.214 | 1.00 | 25.04 |
| 6088 | CB | HIS | B | 123 | 6.888 | 28.867 | 12.233 | 1.00 | 25.27 |
| 6091 | CG | HIS | B | 123 | 6.649 | 29.828 | 11.116 | 1.00 | 25.24 |
| 6092 | ND1 | HIS | B | 123 | 5.983 | 31.018 | 11.293 | 1.00 | 26.70 |
| 6094 | CE1 | HIS | B | 123 | 5.924 | 31.663 | 10.141 | 1.00 | 27.42 |
| 6096 | NE2 | HIS | B | 123 | 6.532 | 30.935 | 9.226 | 1.00 | 26.41 |
| 6098 | CD2 | HIS | B | 123 | 6.985 | 29.776 | 9.807 | 1.00 | 26.27 |
| 6100 | C | HIS | B | 123 | 4.539 | 28.076 | 12.018 | 1.00 | 25.01 |
| 6101 | O | HIS | B | 123 | 3.891 | 28.466 | 12.971 | 1.00 | 25.49 |
| 6102 | N | VAL | B | 124 | 4.051 | 28.021 | 10.784 | 1.00 | 25.12 |
| 6104 | CA | VAL | B | 124 | 2.631 | 28.253 | 10.508 | 1.00 | 25.25 |
| 6106 | CB | VAL | B | 124 | 2.394 | 28.567 | 9.018 | 1.00 | 25.46 |
| 6108 | CG1 | VAL | B | 124 | 0.884 | 28.609 | 8.673 | 1.00 | 26.21 |
| 6112 | CG2 | VAL | B | 124 | 3.035 | 29.894 | 8.681 | 1.00 | 25.70 |
| 6116 | C | VAL | B | 124 | 1.786 | 27.078 | 10.999 | 1.00 | 25.08 |
| 6117 | O | VAL | B | 124 | 0.821 | 27.285 | 11.720 | 1.00 | 24.86 |
| 6118 | N | LYS | B | 125 | 2.167 | 25.856 | 10.639 | 1.00 | 25.25 |
| 6120 | CA | LYS | B | 125 | 1.439 | 24.654 | 11.042 | 1.00 | 25.87 |
| 6122 | CB | LYS | B | 125 | 1.935 | 23.428 | 10.263 | 1.00 | 26.25 |
| 6125 | CG | LYS | B | 125 | 0.884 | 22.726 | 9.418 | 1.00 | 28.80 |
| 6128 | CD | LYS | B | 125 | -0.165 | 22.025 | 10.250 | 1.00 | 31.95 |
| 6131 | CE | LYS | B | 125 | -0.978 | 21.015 | 9.432 | 1.00 | 33.31 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 6134 | NZ | LYS | B | 125 | -1.864 | 21.671 | 8.417 | 1.00 | 34.97 |
| 6138 | C | LYS | B | 125 | 1.468 | 24.365 | 12.564 | 1.00 | 25.31 |
| 6139 | O | LYS | B | 125 | 0.445 | 24.061 | 13.161 | 1.00 | 24.99 |
| 6140 | N | PHE | B | 126 | 2.626 | 24.488 | 13.193 | 1.00 | 24.69 |
| 6142 | CA | PHE | B | 126 | 2.789 | 24.032 | 14.567 | 1.00 | 24.30 |
| 6144 | CB | PHE | B | 126 | 3.908 | 22.993 | 14.616 | 1.00 | 24.16 |
| 6147 | CG | PHE | B | 126 | 3.639 | 21.763 | 13.799 | 1.00 | 24.65 |
| 6148 | CD1 | PHE | B | 126 | 2.915 | 20.704 | 14.332 | 1.00 | 26.16 |
| 6150 | CE1 | PHE | B | 126 | 2.690 | 19.541 | 13.582 | 1.00 | 25.66 |
| 6152 | CZ | PHE | B | 126 | 3.192 | 19.441 | 12.311 | 1.00 | 25.37 |
| 6154 | CE2 | PHE | B | 126 | 3.930 | 20.494 | 11.767 | 1.00 | 24.54 |
| 6156 | CD2 | PHE | B | 126 | 4.158 | 21.637 | 12.513 | 1.00 | 25.35 |
| 6158 | C | PHE | B | 126 | 3.084 | 25.165 | 15.565 | 1.00 | 23.77 |
| 6159 | O | PHE | B | 126 | 3.155 | 24.927 | 16.752 | 1.00 | 23.66 |
| 6160 | N | GLY | B | 127 | 3.250 | 26.391 | 15.083 | 1.00 | 23.69 |
| 6162 | CA | GLY | B | 127 | 3.622 | 27.516 | 15.935 | 1.00 | 23.51 |
| 6165 | C | GLY | B | 127 | 5.130 | 27.773 | 15.955 | 1.00 | 23.55 |
| 6166 | O | GLY | B | 127 | 5.927 | 26.892 | 15.652 | 1.00 | 22.34 |
| 6167 | N | GLU | B | 128 | 5.518 | 28.986 | 16.320 | 1.00 | 23.70 |
| 6169 | CA | GLU | B | 128 | 6.934 | 29.381 | 16.314 | 1.00 | 24.67 |
| 6171 | CB | GLU | B | 128 | 7.091 | 30.868 | 16.639 | 1.00 | 24.89 |
| 6174 | CG | GLU | B | 128 | 6.990 | 31.777 | 15.427 | 1.00 | 27.84 |
| 6177 | CD | GLU | B | 128 | 7.069 | 33.248 | 15.796 | 1.00 | 30.34 |
| 6178 | OE1 | GLU | B | 128 | 8.174 | 33.721 | 16.136 | 1.00 | 35.10 |
| 6179 | OE2 | GLU | B | 128 | 6.033 | 33.931 | 15.743 | 1.00 | 32.39 |
| 6180 | C | GLU | B | 128 | 7.792 | 28.558 | 17.283 | 1.00 | 24.12 |
| 6181 | O | GLU | B | 128 | 8.925 | 28.199 | 16.955 | 1.00 | 23.74 |
| 6182 | N | ALA | B | 129 | 7.249 | 28.292 | 18.469 | 1.00 | 23.52 |
| 6184 | CA | ALA | B | 129 | 7.968 | 27.587 | 19.526 | 1.00 | 23.88 |
| 6186 | CB | ALA | B | 129 | 7.156 | 27.594 | 20.816 | 1.00 | 23.93 |
| 6190 | C | ALA | B | 129 | 8.287 | 26.159 | 19.098 | 1.00 | 23.98 |
| 6191 | O | ALA | B | 129 | 9.417 | 25.688 | 19.247 | 1.00 | 22.97 |
| 6192 | N | ASN | B | 130 | 7.290 | 25.494 | 18.524 | 1.00 | 23.86 |
| 6194 | CA | ASN | B | 130 | 7.484 | 24.159 | 17.980 | 1.00 | 24.09 |
| 6196 | CB | ASN | B | 130 | 6.165 | 23.561 | 17.486 | 1.00 | 24.26 |
| 6199 | CG | ASN | B | 130 | 5.365 | 22.896 | 18.601 | 1.00 | 26.12 |
| 6200 | OD1 | ASN | B | 130 | 4.125 | 22.946 | 18.602 | 1.00 | 27.70 |
| 6201 | ND2 | ASN | B | 130 | 6.064 | 22.278 | 19.561 | 1.00 | 23.40 |
| 6204 | C | ASN | B | 130 | 8.508 | 24.168 | 16.849 | 1.00 | 23.11 |
| 6205 | O | ASN | B | 130 | 9.294 | 23.250 | 16.750 | 1.00 | 22.29 |
| 6206 | N | ALA | B | 131 | 8.496 | 25.208 | 16.015 | 1.00 | 22.58 |
| 6208 | CA | ALA | B | 131 | 9.430 | 25.303 | 14.896 | 1.00 | 22.31 |
| 6210 | CB | ALA | B | 131 | 9.043 | 26.425 | 13.953 | 1.00 | 23.02 |
| 6214 | C | ALA | B | 131 | 10.836 | 25.526 | 15.405 | 1.00 | 21.81 |
| 6215 | O | ALA | B | 131 | 11.766 | 24.906 | 14.932 | 1.00 | 21.37 |
| 6216 | N | ILE | B | 132 | 10.985 | 26.419 | 16.371 | 1.00 | 21.15 |
| 6218 | CA | ILE | B | 132 | 12.293 | 26.701 | 16.936 | 1.00 | 20.84 |
| 6220 | CB | ILE | B | 132 | 12.177 | 27.795 | 18.007 | 1.00 | 20.71 |
| 6222 | CG1 | ILE | B | 132 | 11.994 | 29.168 | 17.339 | 1.00 | 21.50 |
| 6225 | CD1 | ILE | B | 132 | 11.342 | 30.199 | 18.243 | 1.00 | 22.29 |
| 6229 | CG2 | ILE | B | 132 | 13.395 | 27.816 | 18.903 | 1.00 | 21.11 |
| 6233 | C | ILE | B | 132 | 12.888 | 25.423 | 17.523 | 1.00 | 19.99 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 6234 | O | ILE | B | 132 | 14.037 | 25.072 | 17.234 | 1.00 | 19.91 |
| 6235 | N | LEU | B | 133 | 12.094 | 24.746 | 18.342 | 1.00 | 19.38 |
| 6237 | CA | LEU | B | 133 | 12.522 | 23.553 | 19.061 | 1.00 | 19.20 |
| 6239 | CB | LEU | B | 133 | 11.477 | 23.141 | 20.106 | 1.00 | 19.23 |
| 6242 | CG | LEU | B | 133 | 11.417 | 24.029 | 21.357 | 1.00 | 20.75 |
| 6244 | CD1 | LEU | B | 133 | 12.776 | 24.131 | 22.047 | 1.00 | 22.13 |
| 6248 | CD2 | LEU | B | 133 | 10.382 | 23.528 | 22.321 | 1.00 | 22.65 |
| 6252 | C | LEU | B | 133 | 12.776 | 22.413 | 18.096 | 1.00 | 19.26 |
| 6253 | O | LEU | B | 133 | 13.757 | 21.682 | 18.244 | 1.00 | 19.51 |
| 6254 | N | ALA | B | 134 | 11.926 | 22.286 | 17.082 | 1.00 | 18.61 |
| 6256 | CA | ALA | B | 134 | 12.073 | 21.218 | 16.108 | 1.00 | 19.13 |
| 6258 | CB | ALA | B | 134 | 10.873 | 21.183 | 15.181 | 1.00 | 18.64 |
| 6262 | C | ALA | B | 134 | 13.373 | 21.368 | 15.315 | 1.00 | 18.57 |
| 6263 | O | ALA | B | 134 | 14.079 | 20.387 | 15.065 | 1.00 | 18.99 |
| 6264 | N | GLY | B | 135 | 13.685 | 22.595 | 14.916 | 1.00 | 18.91 |
| 6266 | CA | GLY | B | 135 | 14.948 | 22.879 | 14.272 | 1.00 | 18.59 |
| 6269 | C | GLY | B | 135 | 16.117 | 22.574 | 15.200 | 1.00 | 18.99 |
| 6270 | O | GLY | B | 135 | 17.098 | 21.959 | 14.790 | 1.00 | 18.66 |
| 6271 | N | ASP | B | 136 | 16.001 | 22.986 | 16.459 | 1.00 | 19.11 |
| 6273 | CA | ASP | B | 136 | 17.061 | 22.771 | 17.457 | 1.00 | 19.02 |
| 6275 | CB | ASP | B | 136 | 16.652 | 23.327 | 18.829 | 1.00 | 18.48 |
| 6278 | CG | ASP | B | 136 | 16.654 | 24.851 | 18.881 | 1.00 | 20.10 |
| 6279 | OD1 | ASP | B | 136 | 17.086 | 25.482 | 17.880 | 1.00 | 19.13 |
| 6280 | OD2 | ASP | B | 136 | 16.221 | 25.488 | 19.889 | 1.00 | 20.44 |
| 6281 | C | ASP | B | 136 | 17.344 | 21.283 | 17.586 | 1.00 | 18.66 |
| 6282 | O | ASP | B | 136 | 18.481 | 20.860 | 17.541 | 1.00 | 18.36 |
| 6283 | N | ALA | B | 137 | 16.274 | 20.506 | 17.675 | 1.00 | 18.43 |
| 6285 | CA | ALA | B | 137 | 16.347 | 19.069 | 17.878 | 1.00 | 18.51 |
| 6287 | CB | ALA | B | 137 | 15.012 | 18.540 | 18.344 | 1.00 | 18.33 |
| 6291 | C | ALA | B | 137 | 16.808 | 18.315 | 16.629 | 1.00 | 18.44 |
| 6292 | O | ALA | B | 137 | 17.407 | 17.248 | 16.748 | 1.00 | 18.67 |
| 6293 | N | LEU | B | 138 | 16.518 | 18.850 | 15.445 | 1.00 | 18.17 |
| 6295 | CA | LEU | B | 138 | 16.970 | 18.235 | 14.207 | 1.00 | 18.20 |
| 6297 | CB | LEU | B | 138 | 16.213 | 18.786 | 12.995 | 1.00 | 18.38 |
| 6300 | CG | LEU | B | 138 | 14.853 | 18.138 | 12.732 | 1.00 | 17.74 |
| 6302 | CD1 | LEU | B | 138 | 14.127 | 18.905 | 11.651 | 1.00 | 17.44 |
| 6306 | CD2 | LEU | B | 138 | 15.017 | 16.674 | 12.341 | 1.00 | 18.02 |
| 6310 | C | LEU | B | 138 | 18.467 | 18.452 | 14.034 | 1.00 | 18.06 |
| 6311 | O | LEU | B | 138 | 19.167 | 17.572 | 13.544 | 1.00 | 18.16 |
| 6312 | N | GLN | B | 139 | 18.969 | 19.610 | 14.447 | 1.00 | 17.91 |
| 6314 | CA | GLN | B | 139 | 20.412 | 19.804 | 14.412 | 1.00 | 18.74 |
| 6316 | CB | GLN | B | 139 | 20.838 | 21.223 | 14.800 | 1.00 | 18.78 |
| 6319 | CG | GLN | B | 139 | 22.358 | 21.369 | 14.668 | 1.00 | 21.69 |
| 6322 | CD | GLN | B | 139 | 22.953 | 22.631 | 15.232 | 1.00 | 23.34 |
| 6323 | OE1 | GLN | B | 139 | 22.274 | 23.644 | 15.458 | 1.00 | 24.32 |
| 6324 | NE2 | GLN | B | 139 | 24.255 | 22.578 | 15.452 | 1.00 | 26.40 |
| 6327 | C | GLN | B | 139 | 21.094 | 18.762 | 15.319 | 1.00 | 18.33 |
| 6328 | O | GLN | B | 139 | 22.086 | 18.144 | 14.926 | 1.00 | 18.38 |
| 6329 | N | THR | B | 140 | 20.542 | 18.560 | 16.508 | 1.00 | 17.86 |
| 6331 | CA | THR | B | 140 | 21.121 | 17.657 | 17.476 | 1.00 | 18.15 |
| 6333 | CB | THR | B | 140 | 20.384 | 17.734 | 18.820 | 1.00 | 18.21 |
| 6335 | OG1 | THR | B | 140 | 20.296 | 19.101 | 19.283 | 1.00 | 18.94 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 6337 | CG2 | THR | B | 140 | 21.169 | 17.017 | 19.864 | 1.00 | 19.06 |
| 6341 | C | THR | B | 140 | 21.060 | 16.225 | 16.950 | 1.00 | 18.22 |
| 6342 | O | THR | B | 140 | 22.014 | 15.474 | 17.106 | 1.00 | 18.09 |
| 6343 | N | LEU | B | 141 | 19.936 | 15.870 | 16.322 | 1.00 | 17.83 |
| 6345 | CA | LEU | B | 141 | 19.739 | 14.530 | 15.781 | 1.00 | 17.43 |
| 6347 | CB | LEU | B | 141 | 18.336 | 14.416 | 15.184 | 1.00 | 17.61 |
| 6350 | CG | LEU | B | 141 | 18.006 | 13.113 | 14.455 | 1.00 | 18.78 |
| 6352 | CD1 | LEU | B | 141 | 18.167 | 11.908 | 15.367 | 1.00 | 18.23 |
| 6356 | CD2 | LEU | B | 141 | 16.619 | 13.201 | 13.912 | 1.00 | 19.31 |
| 6360 | C | LEU | B | 141 | 20.818 | 14.186 | 14.743 | 1.00 | 16.77 |
| 6361 | O | LEU | B | 141 | 21.287 | 13.045 | 14.664 | 1.00 | 16.01 |
| 6362 | N | ALA | B | 142 | 21.243 | 15.179 | 13.970 | 1.00 | 16.82 |
| 6364 | CA | ALA | B | 142 | 22.280 | 14.960 | 12.974 | 1.00 | 16.89 |
| 6366 | CB | ALA | B | 142 | 22.581 | 16.241 | 12.231 | 1.00 | 17.47 |
| 6370 | C | ALA | B | 142 | 23.548 | 14.406 | 13.625 | 1.00 | 17.27 |
| 6371 | O | ALA | B | 142 | 24.184 | 13.484 | 13.091 | 1.00 | 17.46 |
| 6372 | N | PHE | B | 143 | 23.888 | 14.943 | 14.789 | 1.00 | 17.08 |
| 6374 | CA | PHE | B | 143 | 25.088 | 14.528 | 15.496 | 1.00 | 17.65 |
| 6376 | CB | PHE | B | 143 | 25.593 | 15.666 | 16.381 | 1.00 | 18.03 |
| 6379 | CG | PHE | B | 143 | 26.007 | 16.880 | 15.584 | 1.00 | 18.67 |
| 6380 | CD1 | PHE | B | 143 | 25.230 | 18.019 | 15.566 | 1.00 | 18.86 |
| 6382 | CE1 | PHE | B | 143 | 25.605 | 19.122 | 14.809 | 1.00 | 19.97 |
| 6384 | CZ | PHE | B | 143 | 26.757 | 19.070 | 14.029 | 1.00 | 19.23 |
| 6386 | CE2 | PHE | B | 143 | 27.526 | 17.940 | 14.023 | 1.00 | 19.82 |
| 6388 | CD2 | PHE | B | 143 | 27.140 | 16.835 | 14.788 | 1.00 | 21.06 |
| 6390 | C | PHE | B | 143 | 24.848 | 13.218 | 16.260 | 1.00 | 17.89 |
| 6391 | O | PHE | B | 143 | 25.764 | 12.440 | 16.419 | 1.00 | 17.92 |
| 6392 | N | SER | B | 144 | 23.613 | 12.966 | 16.699 | 1.00 | 18.09 |
| 6394 | CA | SER | B | 144 | 23.275 | 11.661 | 17.269 | 1.00 | 18.71 |
| 6396 | CB | SER | B | 144 | 21.839 | 11.634 | 17.769 | 1.00 | 18.28 |
| 6399 | OG | SER | B | 144 | 21.712 | 12.386 | 18.950 | 1.00 | 19.32 |
| 6401 | C | SER | B | 144 | 23.466 | 10.571 | 16.212 | 1.00 | 18.94 |
| 6402 | O | SER | B | 144 | 24.084 | 9.555 | 16.485 | 1.00 | 19.25 |
| 6403 | N | ILE | B | 145 | 22.967 | 10.819 | 15.001 | 1.00 | 19.22 |
| 6405 | CA | ILE | B | 145 | 23.123 | 9.884 | 13.890 | 1.00 | 19.25 |
| 6407 | CB | ILE | B | 145 | 22.430 | 10.403 | 12.622 | 1.00 | 19.39 |
| 6409 | CG1 | ILE | B | 145 | 20.916 | 10.363 | 12.822 | 1.00 | 18.95 |
| 6412 | CD1 | ILE | B | 145 | 20.144 | 11.100 | 11.805 | 1.00 | 21.43 |
| 6416 | CG2 | ILE | B | 145 | 22.848 | 9.571 | 11.387 | 1.00 | 17.88 |
| 6420 | C | ILE | B | 145 | 24.606 | 9.609 | 13.612 | 1.00 | 19.87 |
| 6421 | O | ILE | B | 145 | 25.021 | 8.461 | 13.593 | 1.00 | 19.68 |
| 6422 | N | LEU | B | 146 | 25.397 | 10.648 | 13.393 | 1.00 | 19.88 |
| 6424 | CA | LEU | B | 146 | 26.799 | 10.451 | 13.025 | 1.00 | 20.40 |
| 6426 | CB | LEU | B | 146 | 27.452 | 11.764 | 12.620 | 1.00 | 20.25 |
| 6429 | CG | LEU | B | 146 | 27.071 | 12.298 | 11.246 | 1.00 | 20.51 |
| 6431 | CD1 | LEU | B | 146 | 27.798 | 13.593 | 11.005 | 1.00 | 23.24 |
| 6435 | CD2 | LEU | B | 146 | 27.402 | 11.299 | 10.149 | 1.00 | 21.98 |
| 6439 | C | LEU | B | 146 | 27.600 | 9.803 | 14.145 | 1.00 | 20.89 |
| 6440 | O | LEU | B | 146 | 28.572 | 9.088 | 13.876 | 1.00 | 21.00 |
| 6441 | N | SER | B | 147 | 27.211 | 10.045 | 15.396 | 1.00 | 21.26 |
| 6443 | CA | SER | B | 147 | 27.933 | 9.439 | 16.514 | 1.00 | 22.16 |
| 6445 | CB | SER | B | 147 | 27.926 | 10.329 | 17.756 | 1.00 | 21.93 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 6448 | OG | SER | B | 147 | 26.615 | 10.552 | 18.225 | 1.00 | 23.99 |
| 6450 | C | SER | B | 147 | 27.456 | 8.023 | 16.856 | 1.00 | 22.90 |
| 6451 | O | SER | B | 147 | 28.248 | 7.250 | 17.390 | 1.00 | 22.85 |
| 6452 | N | ASP | B | 148 | 26.203 | 7.678 | 16.538 | 1.00 | 23.91 |
| 6454 | CA | ASP | B | 148 | 25.580 | 6.411 | 16.991 | 1.00 | 24.85 |
| 6456 | CB | ASP | B | 148 | 24.270 | 6.674 | 17.745 | 1.00 | 25.39 |
| 6459 | CG | ASP | B | 148 | 24.464 | 7.509 | 18.995 | 1.00 | 26.64 |
| 6460 | OD1 | ASP | B | 148 | 23.535 | 8.249 | 19.365 | 1.00 | 25.98 |
| 6461 | OD2 | ASP | B | 148 | 25.516 | 7.497 | 19.667 | 1.00 | 29.60 |
| 6462 | C | ASP | B | 148 | 25.262 | 5.407 | 15.890 | 1.00 | 25.42 |
| 6463 | O | ASP | B | 148 | 25.185 | 4.202 | 16.158 | 1.00 | 25.21 |
| 6464 | N | ALA | B | 149 | 25.052 | 5.887 | 14.663 | 1.00 | 25.69 |
| 6466 | CA | ALA | B | 149 | 24.533 | 5.031 | 13.592 | 1.00 | 26.20 |
| 6468 | CB | ALA | B | 149 | 24.187 | 5.840 | 12.367 | 1.00 | 26.13 |
| 6472 | C | ALA | B | 149 | 25.542 | 3.965 | 13.226 | 1.00 | 26.52 |
| 6473 | O | ALA | B | 149 | 26.739 | 4.190 | 13.292 | 1.00 | 26.08 |
| 6474 | N | ASP | B | 150 | 25.051 | 2.790 | 12.862 | 1.00 | 27.00 |
| 6476 | CA | ASP | B | 150 | 25.908 | 1.760 | 12.308 | 1.00 | 27.79 |
| 6478 | CB | ASP | B | 150 | 25.084 | 0.487 | 12.088 | 1.00 | 28.61 |
| 6481 | CG | ASP | B | 150 | 25.935 | -0.733 | 11.853 | 1.00 | 30.23 |
| 6482 | OD1 | ASP | B | 150 | 27.147 | -0.714 | 12.160 | 1.00 | 33.26 |
| 6483 | OD2 | ASP | B | 150 | 25.452 | -1.776 | 11.358 | 1.00 | 34.68 |
| 6484 | C | ASP | B | 150 | 26.531 | 2.247 | 10.992 | 1.00 | 27.76 |
| 6485 | O | ASP | B | 150 | 25.825 | 2.652 | 10.050 | 1.00 | 27.93 |
| 6486 | N | MET | B | 151 | 27.856 | 2.247 | 10.951 | 1.00 | 27.25 |
| 6488 | CA | MET | B | 151 | 28.612 | 2.526 | 9.743 | 1.00 | 27.33 |
| 6490 | CB | MET | B | 151 | 29.181 | 3.936 | 9.772 | 1.00 | 26.88 |
| 6493 | CG | MET | B | 151 | 28.129 | 5.014 | 9.664 | 1.00 | 26.79 |
| 6496 | SD | MET | B | 151 | 28.859 | 6.646 | 9.270 | 1.00 | 27.26 |
| 6497 | CE | MET | B | 151 | 29.830 | 6.916 | 10.701 | 1.00 | 23.05 |
| 6501 | C | MET | B | 151 | 29.737 | 1.508 | 9.657 | 1.00 | 27.62 |
| 6502 | O | MET | B | 151 | 30.895 | 1.812 | 9.936 | 1.00 | 26.26 |
| 6503 | N | PRO | B | 152 | 29.393 | 0.291 | 9.256 | 1.00 | 28.79 |
| 6504 | CA | PRO | B | 152 | 30.354 | -0.815 | 9.234 | 1.00 | 29.73 |
| 6506 | CB | PRO | B | 152 | 29.669 | -1.832 | 8.320 | 1.00 | 29.99 |
| 6509 | CG | PRO | B | 152 | 28.228 | -1.630 | 8.593 | 1.00 | 29.30 |
| 6512 | CD | PRO | B | 152 | 28.060 | -0.137 | 8.799 | 1.00 | 29.11 |
| 6515 | C | PRO | B | 152 | 31.733 | -0.464 | 8.696 | 1.00 | 30.46 |
| 6516 | O | PRO | B | 152 | 32.732 | -0.822 | 9.317 | 1.00 | 30.83 |
| 6517 | N | GLU | B | 153 | 31.801 | 0.253 | 7.586 | 1.00 | 31.81 |
| 6519 | CA | GLU | B | 153 | 33.089 | 0.431 | 6.905 | 1.00 | 33.36 |
| 6521 | CB | GLU | B | 153 | 32.889 | 0.840 | 5.426 | 1.00 | 34.57 |
| 6524 | CG | GLU | B | 153 | 31.629 | 0.304 | 4.730 | 1.00 | 37.40 |
| 6527 | CD | GLU | B | 153 | 31.768 | 0.264 | 3.209 | 1.00 | 41.76 |
| 6528 | OE1 | GLU | B | 153 | 30.918 | -0.387 | 2.543 | 1.00 | 42.19 |
| 6529 | OE2 | GLU | B | 153 | 32.733 | 0.877 | 2.676 | 1.00 | 43.49 |
| 6530 | C | GLU | B | 153 | 34.030 | 1.449 | 7.587 | 1.00 | 32.65 |
| 6531 | O | GLU | B | 153 | 35.172 | 1.605 | 7.155 | 1.00 | 33.17 |
| 6532 | N | VAL | B | 154 | 33.572 | 2.099 | 8.660 | 1.00 | 31.25 |
| 6534 | CA | VAL | B | 154 | 34.097 | 3.410 | 9.043 | 1.00 | 30.18 |
| 6536 | CB | VAL | B | 154 | 32.970 | 4.456 | 9.012 | 1.00 | 30.21 |
| 6538 | CG1 | VAL | B | 154 | 33.501 | 5.842 | 9.381 | 1.00 | 29.95 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 6542 | CG2 | VAL | B | 154 | 32.310 | 4.467 | 7.634 | 1.00 | 30.63 |
| 6546 | C | VAL | B | 154 | 34.767 | 3.425 | 10.417 | 1.00 | 28.89 |
| 6547 | O | VAL | B | 154 | 34.131 | 3.174 | 11.431 | 1.00 | 27.43 |
| 6548 | N | SER | B | 155 | 36.057 | 3.755 | 10.435 | 1.00 | 28.02 |
| 6550 | CA | SER | B | 155 | 36.806 | 3.836 | 11.681 | 1.00 | 27.32 |
| 6552 | CB | SER | B | 155 | 38.302 | 4.022 | 11.413 | 1.00 | 27.23 |
| 6555 | OG | SER | B | 155 | 38.554 | 5.276 | 10.811 | 1.00 | 25.67 |
| 6557 | C | SER | B | 155 | 36.295 | 4.984 | 12.540 | 1.00 | 27.03 |
| 6558 | O | SER | B | 155 | 35.651 | 5.906 | 12.045 | 1.00 | 26.50 |
| 6559 | N | ASP | B | 156 | 36.601 | 4.899 | 13.831 | 1.00 | 26.71 |
| 6561 | CA | ASP | B | 156 | 36.236 | 5.914 | 14.810 | 1.00 | 26.65 |
| 6563 | CB | ASP | B | 156 | 36.729 | 5.509 | 16.194 | 1.00 | 26.35 |
| 6566 | CG | ASP | B | 156 | 35.776 | 4.575 | 16.906 | 1.00 | 28.03 |
| 6567 | OD1 | ASP | B | 156 | 36.086 | 4.216 | 18.054 | 1.00 | 30.17 |
| 6568 | OD2 | ASP | B | 156 | 34.692 | 4.157 | 16.424 | 1.00 | 29.62 |
| 6569 | C | ASP | B | 156 | 36.824 | 7.253 | 14.407 | 1.00 | 26.23 |
| 6570 | O | ASP | B | 156 | 36.146 | 8.269 | 14.454 | 1.00 | 25.29 |
| 6571 | N | ARG | B | 157 | 38.077 | 7.229 | 13.970 | 1.00 | 26.28 |
| 6573 | CA | ARG | B | 157 | 38.745 | 8.409 | 13.442 | 1.00 | 26.55 |
| 6575 | CB | ARG | B | 157 | 40.172 | 8.069 | 13.019 | 1.00 | 27.45 |
| 6578 | CG | ARG | B | 157 | 41.099 | 9.254 | 13.054 | 1.00 | 30.78 |
| 6581 | CD | ARG | B | 157 | 41.726 | 9.500 | 14.416 | 1.00 | 34.73 |
| 6584 | NE | ARG | B | 157 | 41.001 | 10.520 | 15.179 | 1.00 | 38.97 |
| 6586 | CZ | ARG | B | 157 | 41.152 | 11.835 | 15.043 | 1.00 | 42.64 |
| 6587 | NH1 | ARG | B | 157 | 42.000 | 12.354 | 14.148 | 1.00 | 45.06 |
| 6590 | NH2 | ARG | B | 157 | 40.435 | 12.651 | 15.801 | 1.00 | 43.15 |
| 6593 | C | ARG | B | 157 | 38.004 | 9.052 | 12.268 | 1.00 | 25.50 |
| 6594 | O | ARG | B | 157 | 37.870 | 10.265 | 12.211 | 1.00 | 25.19 |
| 6595 | N | ASP | B | 158 | 37.540 | 8.252 | 11.315 | 1.00 | 24.83 |
| 6597 | CA | ASP | B | 158 | 36.823 | 8.813 | 10.171 | 1.00 | 24.18 |
| 6599 | CB | ASP | B | 158 | 36.747 | 7.809 | 9.030 | 1.00 | 24.78 |
| 6602 | CG | ASP | B | 158 | 38.117 | 7.499 | 8.443 | 1.00 | 26.32 |
| 6603 | OD1 | ASP | B | 158 | 39.074 | 8.280 | 8.679 | 1.00 | 29.38 |
| 6604 | OD2 | ASP | B | 158 | 38.329 | 6.479 | 7.758 | 1.00 | 28.43 |
| 6605 | C | ASP | B | 158 | 35.427 | 9.290 | 10.562 | 1.00 | 22.75 |
| 6606 | O | ASP | B | 158 | 34.923 | 10.240 | 10.007 | 1.00 | 22.39 |
| 6607 | N | ARG | B | 159 | 34.810 | 8.619 | 11.521 | 1.00 | 21.86 |
| 6609 | CA | ARG | B | 159 | 33.532 | 9.053 | 12.064 | 1.00 | 20.79 |
| 6611 | CB | ARG | B | 159 | 33.022 | 8.054 | 13.088 | 1.00 | 20.74 |
| 6614 | CG | ARG | B | 159 | 31.647 | 8.375 | 13.651 | 1.00 | 20.82 |
| 6617 | CD | ARG | B | 159 | 31.205 | 7.399 | 14.704 | 1.00 | 20.94 |
| 6620 | NE | ARG | B | 159 | 30.980 | 6.045 | 14.173 | 1.00 | 22.48 |
| 6622 | CZ | ARG | B | 159 | 29.790 | 5.511 | 13.895 | 1.00 | 23.71 |
| 6623 | NH1 | ARG | B | 159 | 29.723 | 4.256 | 13.448 | 1.00 | 25.23 |
| 6626 | NH2 | ARG | B | 159 | 28.671 | 6.205 | 14.046 | 1.00 | 20.67 |
| 6629 | C | ARG | B | 159 | 33.676 | 10.426 | 12.714 | 1.00 | 20.58 |
| 6630 | O | ARG | B | 159 | 32.833 | 11.297 | 12.519 | 1.00 | 18.98 |
| 6631 | N | ILE | B | 160 | 34.752 | 10.610 | 13.483 | 1.00 | 20.29 |
| 6633 | CA | ILE | B | 160 | 35.016 | 11.891 | 14.124 | 1.00 | 20.38 |
| 6635 | CB | ILE | B | 160 | 36.209 | 11.808 | 15.090 | 1.00 | 20.21 |
| 6637 | CG1 | ILE | B | 160 | 35.848 | 10.962 | 16.319 | 1.00 | 20.02 |
| 6640 | CD1 | ILE | B | 160 | 37.077 | 10.390 | 17.035 | 1.00 | 21.78 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 6644 | CG2 | ILE | B | 160 | 36.656 | 13.203 | 15.514 | 1.00 | 21.46 |
| 6648 | C | ILE | B | 160 | 35.247 | 12.940 | 13.051 | 1.00 | 20.53 |
| 6649 | O | ILE | B | 160 | 34.737 | 14.018 | 13.158 | 1.00 | 20.41 |
| 6650 | N | SER | B | 161 | 35.976 | 12.593 | 11.996 | 1.00 | 21.07 |
| 6652 | CA | SER | B | 161 | 36.182 | 13.485 | 10.864 | 1.00 | 21.78 |
| 6654 | CB | SER | B | 161 | 37.097 | 12.822 | 9.824 | 1.00 | 22.36 |
| 6657 | OG | SER | B | 161 | 38.452 | 13.117 | 10.107 | 1.00 | 25.91 |
| 6659 | C | SER | B | 161 | 34.867 | 13.924 | 10.186 | 1.00 | 21.46 |
| 6660 | O | SER | B | 161 | 34.771 | 15.053 | 9.711 | 1.00 | 21.56 |
| 6661 | N | MET | B | 162 | 33.886 | 13.029 | 10.125 | 1.00 | 21.47 |
| 6663 | CA | MET | B | 162 | 32.569 | 13.337 | 9.576 | 1.00 | 21.23 |
| 6665 | CB | MET | B | 162 | 31.726 | 12.079 | 9.403 | 1.00 | 21.94 |
| 6668 | CG | MET | B | 162 | 32.183 | 11.183 | 8.281 | 1.00 | 24.79 |
| 6671 | SD | MET | B | 162 | 31.189 | 9.677 | 8.224 | 1.00 | 31.73 |
| 6672 | CE | MET | B | 162 | 32.337 | 8.674 | 7.553 | 1.00 | 32.04 |
| 6676 | C | MET | B | 162 | 31.815 | 14.278 | 10.480 | 1.00 | 20.18 |
| 6677 | O | MET | B | 162 | 31.164 | 15.191 | 10.005 | 1.00 | 20.12 |
| 6678 | N | ILE | B | 163 | 31.894 | 14.045 | 11.782 | 1.00 | 20.00 |
| 6680 | CA | ILE | B | 163 | 31.238 | 14.915 | 12.744 | 1.00 | 19.69 |
| 6682 | CB | ILE | B | 163 | 31.290 | 14.326 | 14.178 | 1.00 | 19.62 |
| 6684 | CG1 | ILE | B | 163 | 30.466 | 13.047 | 14.259 | 1.00 | 19.47 |
| 6687 | CD1 | ILE | B | 163 | 30.741 | 12.182 | 15.483 | 1.00 | 21.29 |
| 6691 | CG2 | ILE | B | 163 | 30.763 | 15.332 | 15.177 | 1.00 | 18.69 |
| 6695 | C | ILE | B | 163 | 31.878 | 16.289 | 12.688 | 1.00 | 19.80 |
| 6696 | O | ILE | B | 163 | 31.182 | 17.300 | 12.684 | 1.00 | 20.00 |
| 6697 | N | SER | B | 164 | 33.204 | 16.340 | 12.640 | 1.00 | 19.73 |
| 6699 | CA | SER | B | 164 | 33.894 | 17.619 | 12.559 | 1.00 | 19.44 |
| 6701 | CB | SER | B | 164 | 35.410 | 17.419 | 12.507 | 1.00 | 19.53 |
| 6704 | OG | SER | B | 164 | 36.053 | 18.665 | 12.347 | 1.00 | 19.74 |
| 6706 | C | SER | B | 164 | 33.469 | 18.403 | 11.325 | 1.00 | 19.46 |
| 6707 | O | SER | B | 164 | 33.193 | 19.587 | 11.408 | 1.00 | 18.61 |
| 6708 | N | GLU | B | 165 | 33.429 | 17.734 | 10.181 | 1.00 | 20.02 |
| 6710 | CA | GLU | B | 165 | 33.084 | 18.384 | 8.932 | 1.00 | 20.06 |
| 6712 | CB | GLU | B | 165 | 33.224 | 17.423 | 7.757 | 1.00 | 20.49 |
| 6715 | CG | GLU | B | 165 | 32.576 | 17.922 | 6.472 | 1.00 | 21.89 |
| 6718 | CD | GLU | B | 165 | 33.103 | 19.290 | 6.041 | 1.00 | 23.61 |
| 6719 | OE1 | GLU | B | 165 | 34.281 | 19.584 | 6.322 | 1.00 | 24.99 |
| 6720 | OE2 | GLU | B | 165 | 32.347 | 20.067 | 5.426 | 1.00 | 25.28 |
| 6721 | C | GLU | B | 165 | 31.658 | 18.934 | 8.990 | 1.00 | 19.72 |
| 6722 | O | GLU | B | 165 | 31.422 | 20.062 | 8.577 | 1.00 | 19.69 |
| 6723 | N | LEU | B | 166 | 30.720 | 18.140 | 9.494 | 1.00 | 18.90 |
| 6725 | CA | LEU | B | 166 | 29.324 | 18.550 | 9.526 | 1.00 | 18.94 |
| 6727 | CB | LEU | B | 166 | 28.406 | 17.404 | 9.956 | 1.00 | 18.87 |
| 6730 | CG | LEU | B | 166 | 26.915 | 17.695 | 9.771 | 1.00 | 19.53 |
| 6732 | CD1 | LEU | B | 166 | 26.644 | 18.166 | 8.357 | 1.00 | 19.83 |
| 6736 | CD2 | LEU | B | 166 | 26.076 | 16.470 | 10.093 | 1.00 | 20.63 |
| 6740 | C | LEU | B | 166 | 29.158 | 19.736 | 10.458 | 1.00 | 18.48 |
| 6741 | O | LEU | B | 166 | 28.486 | 20.694 | 10.130 | 1.00 | 18.99 |
| 6742 | N | ALA | B | 167 | 29.803 | 19.673 | 11.612 | 1.00 | 18.69 |
| 6744 | CA | ALA | B | 167 | 29.769 | 20.773 | 12.560 | 1.00 | 18.51 |
| 6746 | CB | ALA | B | 167 | 30.446 | 20.384 | 13.872 | 1.00 | 18.21 |
| 6750 | C | ALA | B | 167 | 30.377 | 22.045 | 11.970 | 1.00 | 19.04 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 6751 | O | ALA | B | 167 | 29.749 | 23.095 | 12.012 | 1.00 | 18.97 |
| 6752 | N | SER | B | 168 | 31.573 | 21.976 | 11.387 | 1.00 | 19.49 |
| 6754 | CA | SER | B | 168 | 32.161 | 23.190 | 10.838 | 1.00 | 19.97 |
| 6756 | CB | SER | B | 168 | 33.630 | 22.988 | 10.472 | 1.00 | 20.60 |
| 6759 | OG | SER | B | 168 | 33.756 | 21.975 | 9.518 | 1.00 | 24.18 |
| 6761 | C | SER | B | 168 | 31.348 | 23.734 | 9.643 | 1.00 | 19.40 |
| 6762 | O | SER | B | 168 | 31.186 | 24.958 | 9.482 | 1.00 | 18.70 |
| 6763 | N | ALA | B | 169 | 30.813 | 22.832 | 8.825 | 1.00 | 19.19 |
| 6765 | CA | ALA | B | 169 | 29.974 | 23.225 | 7.690 | 1.00 | 18.98 |
| 6767 | CB | ALA | B | 169 | 29.671 | 22.011 | 6.798 | 1.00 | 19.19 |
| 6771 | C | ALA | B | 169 | 28.672 | 23.907 | 8.081 | 1.00 | 18.85 |
| 6772 | O | ALA | B | 169 | 28.157 | 24.742 | 7.341 | 1.00 | 19.30 |
| 6773 | N | SER | B | 170 | 28.135 | 23.537 | 9.228 | 1.00 | 18.81 |
| 6775 | CA | SER | B | 170 | 26.788 | 23.931 | 9.638 | 1.00 | 18.52 |
| 6777 | CB | SER | B | 170 | 26.128 | 22.787 | 10.405 | 1.00 | 18.45 |
| 6780 | OG | SER | B | 170 | 26.073 | 21.610 | 9.622 | 1.00 | 18.06 |
| 6782 | C | SER | B | 170 | 26.780 | 25.159 | 10.526 | 1.00 | 18.48 |
| 6783 | O | SER | B | 170 | 25.779 | 25.828 | 10.630 | 1.00 | 18.20 |
| 6784 | N | GLY | B | 171 | 27.902 | 25.438 | 11.177 | 1.00 | 19.42 |
| 6786 | CA | GLY | B | 171 | 27.950 | 26.481 | 12.175 | 1.00 | 19.70 |
| 6789 | C | GLY | B | 171 | 28.359 | 27.810 | 11.598 | 1.00 | 20.33 |
| 6790 | O | GLY | B | 171 | 28.096 | 28.122 | 10.441 | 1.00 | 19.41 |
| 6791 | N | ILE | B | 172 | 29.018 | 28.604 | 12.424 | 1.00 | 21.45 |
| 6793 | CA | ILE | B | 172 | 29.348 | 29.976 | 12.074 | 1.00 | 22.91 |
| 6795 | CB | ILE | B | 172 | 29.846 | 30.707 | 13.354 | 1.00 | 23.50 |
| 6797 | CG1 | ILE | B | 172 | 29.737 | 32.206 | 13.173 | 1.00 | 25.77 |
| 6800 | CD1 | ILE | B | 172 | 28.314 | 32.688 | 13.353 | 1.00 | 25.49 |
| 6804 | CG2 | ILE | B | 172 | 31.229 | 30.245 | 13.727 | 1.00 | 24.89 |
| 6808 | C | ILE | B | 172 | 30.354 | 30.068 | 10.916 | 1.00 | 22.56 |
| 6809 | O | ILE | B | 172 | 30.335 | 31.016 | 10.141 | 1.00 | 22.77 |
| 6810 | N | ALA | B | 173 | 31.207 | 29.059 | 10.771 | 1.00 | 22.49 |
| 6812 | CA | ALA | B | 173 | 32.152 | 29.006 | 9.656 | 1.00 | 22.06 |
| 6814 | CB | ALA | B | 173 | 33.324 | 28.148 | 10.023 | 1.00 | 21.92 |
| 6818 | C | ALA | B | 173 | 31.490 | 28.488 | 8.383 | 1.00 | 22.04 |
| 6819 | O | ALA | B | 173 | 32.146 | 28.318 | 7.376 | 1.00 | 22.97 |
| 6820 | N | GLY | B | 174 | 30.181 | 28.252 | 8.430 | 1.00 | 21.24 |
| 6822 | CA | GLY | B | 174 | 29.464 | 27.684 | 7.313 | 1.00 | 20.53 |
| 6825 | C | GLY | B | 174 | 28.034 | 28.189 | 7.292 | 1.00 | 20.28 |
| 6826 | O | GLY | B | 174 | 27.804 | 29.394 | 7.295 | 1.00 | 19.03 |
| 6827 | N | MET | B | 175 | 27.082 | 27.265 | 7.340 | 1.00 | 20.39 |
| 6829 | CA | MET | B | 175 | 25.676 | 27.559 | 7.077 | 1.00 | 21.14 |
| 6831 | CB | MET | B | 175 | 24.855 | 26.298 | 7.278 | 1.00 | 21.40 |
| 6834 | CG | MET | B | 175 | 23.410 | 26.392 | 6.837 | 1.00 | 23.14 |
| 6837 | SD | MET | B | 175 | 22.401 | 27.153 | 8.090 | 1.00 | 26.74 |
| 6838 | CE | MET | B | 175 | 22.407 | 25.862 | 9.410 | 1.00 | 26.17 |
| 6842 | C | MET | B | 175 | 25.147 | 28.696 | 7.938 | 1.00 | 21.67 |
| 6843 | O | MET | B | 175 | 24.556 | 29.644 | 7.436 | 1.00 | 21.21 |
| 6844 | N | CYS | B | 176 | 25.367 | 28.594 | 9.239 | 1.00 | 22.13 |
| 6846 | CA | CYS | B | 176 | 24.827 | 29.556 | 10.170 | 1.00 | 22.50 |
| 6848 | CB | BCYS | B | 176 | 25.042 | 29.096 | 11.614 | 0.35 | 22.49 |
| 6849 | CB | ACYS | B | 176 | 25.010 | 29.057 | 11.596 | 0.65 | 22.96 |
| 6854 | SG | BCYS | B | 176 | 23.609 | 28.307 | 12.340 | 0.35 | 22.05 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 6855 | SG | ACYS | B | 176 | 24.028 | 29.996 | 12.749 | 0.65 | 25.42 |
| 6856 | C | CYS | B | 176 | 25.460 | 30.935 | 9.997 | 1.00 | 21.94 |
| 6857 | O | CYS | B | 176 | 24.775 | 31.934 | 10.105 | 1.00 | 22.08 |
| 6858 | N | GLY | B | 177 | 26.767 | 30.980 | 9.758 | 1.00 | 21.27 |
| 6860 | CA | GLY | B | 177 | 27.453 | 32.231 | 9.504 | 1.00 | 21.35 |
| 6863 | C | GLY | B | 177 | 26.951 | 32.858 | 8.218 | 1.00 | 20.97 |
| 6864 | O | GLY | B | 177 | 26.839 | 34.081 | 8.111 | 1.00 | 20.81 |
| 6865 | N | GLY | B | 178 | 26.643 | 32.009 | 7.249 | 1.00 | 20.08 |
| 6867 | CA | GLY | B | 178 | 26.027 | 32.440 | 6.009 | 1.00 | 19.62 |
| 6870 | C | GLY | B | 178 | 24.641 | 33.007 | 6.215 | 1.00 | 19.25 |
| 6871 | O | GLY | B | 178 | 24.288 | 34.011 | 5.605 | 1.00 | 18.27 |
| 6872 | N | GLN | B | 179 | 23.858 | 32.380 | 7.084 | 1.00 | 18.75 |
| 6874 | CA | GLN | B | 179 | 22.535 | 32.890 | 7.404 | 1.00 | 19.22 |
| 6876 | CB | GLN | B | 179 | 21.787 | 31.947 | 8.348 | 1.00 | 19.67 |
| 6879 | CG | GLN | B | 179 | 21.349 | 30.652 | 7.682 | 1.00 | 20.18 |
| 6882 | CD | GLN | B | 179 | 20.333 | 30.899 | 6.597 | 1.00 | 20.92 |
| 6883 | OE1 | GLN | B | 179 | 20.701 | 31.297 | 5.496 | 1.00 | 21.77 |
| 6884 | NE2 | GLN | B | 179 | 19.047 | 30.712 | 6.914 | 1.00 | 19.90 |
| 6887 | C | GLN | B | 179 | 22.632 | 34.281 | 8.002 | 1.00 | 19.31 |
| 6888 | O | GLN | B | 179 | 21.805 | 35.146 | 7.691 | 1.00 | 18.98 |
| 6889 | N | ALA | B | 180 | 23.667 | 34.503 | 8.810 | 1.00 | 19.26 |
| 6891 | CA | ALA | B | 180 | 23.894 | 35.813 | 9.437 | 1.00 | 20.09 |
| 6893 | CB | ALA | B | 180 | 24.956 | 35.725 | 10.526 | 1.00 | 19.57 |
| 6897 | C | ALA | B | 180 | 24.292 | 36.845 | 8.387 | 1.00 | 20.47 |
| 6898 | O | ALA | B | 180 | 23.826 | 37.969 | 8.440 | 1.00 | 21.60 |
| 6899 | N | LEU | B | 181 | 25.143 | 36.464 | 7.436 | 1.00 | 21.00 |
| 6901 | CA | LEU | B | 181 | 25.561 | 37.384 | 6.371 | 1.00 | 21.21 |
| 6903 | CB | LEU | B | 181 | 26.646 | 36.753 | 5.497 | 1.00 | 21.41 |
| 6906 | CG | LEU | B | 181 | 28.026 | 36.557 | 6.121 | 1.00 | 23.45 |
| 6908 | CD1 | LEU | B | 181 | 28.948 | 35.855 | 5.138 | 1.00 | 24.47 |
| 6912 | CD2 | LEU | B | 181 | 28.630 | 37.913 | 6.562 | 1.00 | 24.78 |
| 6916 | C | LEU | B | 181 | 24.358 | 37.776 | 5.519 | 1.00 | 21.36 |
| 6917 | O | LEU | B | 181 | 24.210 | 38.942 | 5.118 | 1.00 | 20.88 |
| 6918 | N | ASP | B | 182 | 23.498 | 36.794 | 5.258 | 1.00 | 21.82 |
| 6920 | CA | ASP | B | 182 | 22.291 | 36.980 | 4.466 | 1.00 | 22.30 |
| 6922 | CB | ASP | B | 182 | 21.615 | 35.625 | 4.252 | 1.00 | 22.47 |
| 6925 | CG | ASP | B | 182 | 20.205 | 35.739 | 3.779 | 1.00 | 21.57 |
| 6926 | OD1 | ASP | B | 182 | 19.938 | 35.449 | 2.588 | 1.00 | 22.94 |
| 6927 | OD2 | ASP | B | 182 | 19.281 | 36.072 | 4.540 | 1.00 | 25.04 |
| 6928 | C | ASP | B | 182 | 21.356 | 37.989 | 5.138 | 1.00 | 23.38 |
| 6929 | O | ASP | B | 182 | 20.856 | 38.927 | 4.499 | 1.00 | 23.61 |
| 6930 | N | LEU | B | 183 | 21.131 | 37.814 | 6.429 | 1.00 | 24.61 |
| 6932 | CA | LEU | B | 183 | 20.296 | 38.751 | 7.181 | 1.00 | 26.08 |
| 6934 | CB | LEU | B | 183 | 20.112 | 38.267 | 8.621 | 1.00 | 26.86 |
| 6937 | CG | LEU | B | 183 | 18.842 | 37.475 | 8.968 | 1.00 | 28.65 |
| 6939 | CD1 | LEU | B | 183 | 18.029 | 36.990 | 7.768 | 1.00 | 30.94 |
| 6943 | CD2 | LEU | B | 183 | 19.243 | 36.330 | 9.825 | 1.00 | 29.29 |
| 6947 | C | LEU | B | 183 | 20.891 | 40.147 | 7.193 | 1.00 | 26.38 |
| 6948 | O | LEU | B | 183 | 20.176 | 41.134 | 7.048 | 1.00 | 27.18 |
| 6949 | N | ASP | B | 184 | 22.203 | 40.228 | 7.355 | 1.00 | 27.07 |
| 6951 | CA | ASP | B | 184 | 22.893 | 41.513 | 7.389 | 1.00 | 27.97 |
| 6953 | CB | ASP | B | 184 | 24.336 | 41.337 | 7.864 | 1.00 | 28.49 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 6956 | CG | ASP | B | 184 | 24.926 | 42.624 | 8.427 | 1.00 | 31.55 |
| 6957 | OD1 | ASP | B | 184 | 25.937 | 43.106 | 7.874 | 1.00 | 34.43 |
| 6958 | OD2 | ASP | B | 184 | 24.447 | 43.218 | 9.419 | 1.00 | 36.43 |
| 6959 | C | ASP | B | 184 | 22.865 | 42.228 | 6.034 | 1.00 | 27.98 |
| 6960 | O | ASP | B | 184 | 22.853 | 43.454 | 5.993 | 1.00 | 27.47 |
| 6961 | N | ALA | B | 185 | 22.828 | 41.462 | 4.936 | 1.00 | 27.64 |
| 6963 | CA | ALA | B | 185 | 22.818 | 42.026 | 3.576 | 1.00 | 27.64 |
| 6965 | CB | ALA | B | 185 | 23.397 | 41.024 | 2.579 | 1.00 | 27.26 |
| 6969 | C | ALA | B | 185 | 21.415 | 42.474 | 3.118 | 1.00 | 27.90 |
| 6970 | O | ALA | B | 185 | 21.288 | 43.142 | 2.109 | 1.00 | 27.38 |
| 6971 | N | GLU | B | 186 | 20.374 | 42.097 | 3.852 | 1.00 | 28.50 |
| 6973 | CA | GLU | B | 186 | 19.006 | 42.515 | 3.535 | 1.00 | 29.13 |
| 6975 | CB | GLU | B | 186 | 18.031 | 42.069 | 4.629 | 1.00 | 29.71 |
| 6978 | CG | GLU | B | 186 | 17.071 | 40.969 | 4.234 | 1.00 | 31.66 |
| 6981 | CD | GLU | B | 186 | 16.175 | 40.534 | 5.384 | 1.00 | 33.14 |
| 6982 | OE1 | GLU | B | 186 | 15.509 | 41.400 | 5.995 | 1.00 | 35.30 |
| 6983 | OE2 | GLU | B | 186 | 16.149 | 39.324 | 5.684 | 1.00 | 32.62 |
| 6984 | C | GLU | B | 186 | 18.922 | 44.041 | 3.418 | 1.00 | 29.49 |
| 6985 | O | GLU | B | 186 | 19.290 | 44.755 | 4.348 | 1.00 | 28.60 |
| 6986 | N | GLY | B | 187 | 18.454 | 44.518 | 2.264 | 1.00 | 29.61 |
| 6988 | CA | GLY | B | 187 | 18.279 | 45.935 | 1.997 | 1.00 | 29.83 |
| 6991 | C | GLY | B | 187 | 19.560 | 46.670 | 1.658 | 1.00 | 30.04 |
| 6992 | O | GLY | B | 187 | 19.532 | 47.871 | 1.420 | 1.00 | 30.48 |
| 6993 | N | LYS | B | 188 | 20.681 | 45.954 | 1.622 | 1.00 | 30.21 |
| 6995 | CA | LYS | B | 188 | 21.992 | 46.573 | 1.506 | 1.00 | 30.46 |
| 6997 | CB | LYS | B | 188 | 22.959 | 45.982 | 2.526 | 1.00 | 30.97 |
| 7000 | CG | LYS | B | 188 | 22.593 | 46.287 | 3.973 | 1.00 | 32.58 |
| 7003 | CD | LYS | B | 188 | 23.830 | 46.343 | 4.864 | 1.00 | 34.32 |
| 7006 | CE | LYS | B | 188 | 23.490 | 46.882 | 6.259 | 1.00 | 35.98 |
| 7009 | NZ | LYS | B | 188 | 23.339 | 45.804 | 7.290 | 1.00 | 36.88 |
| 7013 | C | LYS | B | 188 | 22.573 | 46.427 | 0.116 | 1.00 | 30.22 |
| 7014 | O | LYS | B | 188 | 23.559 | 47.083 | -0.203 | 1.00 | 30.23 |
| 7015 | N | HIS | B | 189 | 21.984 | 45.555 | -0.700 | 1.00 | 29.28 |
| 7017 | CA | HIS | B | 189 | 22.375 | 45.441 | -2.093 | 1.00 | 29.34 |
| 7019 | CB | HIS | B | 189 | 21.892 | 46.684 | -2.856 | 1.00 | 29.70 |
| 7022 | CG | HIS | B | 189 | 20.410 | 46.833 | -2.832 | 1.00 | 30.08 |
| 7023 | ND1 | HIS | B | 189 | 19.699 | 47.003 | -1.668 | 1.00 | 32.28 |
| 7025 | CE1 | HIS | B | 189 | 18.412 | 47.068 | -1.942 | 1.00 | 31.16 |
| 7027 | NE2 | HIS | B | 189 | 18.261 | 46.940 | -3.244 | 1.00 | 32.50 |
| 7029 | CD2 | HIS | B | 189 | 19.497 | 46.782 | -3.821 | 1.00 | 32.70 |
| 7031 | C | HIS | B | 189 | 23.887 | 45.297 | -2.191 | 1.00 | 28.93 |
| 7032 | O | HIS | B | 189 | 24.558 | 46.097 | -2.847 | 1.00 | 29.19 |
| 7033 | N | VAL | B | 190 | 24.415 | 44.274 | -1.522 | 1.00 | 27.85 |
| 7035 | CA | VAL | B | 190 | 25.850 | 44.103 | -1.417 | 1.00 | 27.29 |
| 7037 | CB | VAL | B | 190 | 26.247 | 43.065 | -0.319 | 1.00 | 27.33 |
| 7039 | CG1 | VAL | B | 190 | 25.636 | 43.452 | 1.052 | 1.00 | 27.10 |
| 7043 | CG2 | VAL | B | 190 | 25.860 | 41.634 | -0.722 | 1.00 | 27.05 |
| 7047 | C | VAL | B | 190 | 26.419 | 43.723 | -2.779 | 1.00 | 26.86 |
| 7048 | O | VAL | B | 190 | 25.733 | 43.075 | -3.577 | 1.00 | 26.12 |
| 7049 | N | PRO | B | 191 | 27.663 | 44.126 | -3.051 | 1.00 | 26.31 |
| 7050 | CA | PRO | B | 191 | 28.314 | 43.792 | -4.319 | 1.00 | 26.16 |
| 7052 | CB | PRO | B | 191 | 29.596 | 44.623 | -4.284 | 1.00 | 26.24 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 7055 | CG | PRO | B | 191 | 29.892 | 44.801 | -2.835 | 1.00 | 26.65 |
| 7058 | CD | PRO | B | 191 | 28.552 | 44.905 | -2.168 | 1.00 | 26.81 |
| 7061 | C | PRO | B | 191 | 28.646 | 42.297 | -4.436 | 1.00 | 25.85 |
| 7062 | O | PRO | B | 191 | 28.521 | 41.553 | -3.475 | 1.00 | 24.67 |
| 7063 | N | LEU | B | 192 | 29.106 | 41.908 | -5.616 | 1.00 | 26.22 |
| 7065 | CA | LEU | B | 192 | 29.284 | 40.509 | -6.002 | 1.00 | 26.42 |
| 7067 | CB | LEU | B | 192 | 29.859 | 40.422 | -7.424 | 1.00 | 26.65 |
| 7070 | CG | LEU | B | 192 | 29.462 | 39.279 | -8.371 | 1.00 | 28.07 |
| 7072 | CD1 | LEU | B | 192 | 30.565 | 39.033 | -9.399 | 1.00 | 29.61 |
| 7076 | CD2 | LEU | B | 192 | 29.105 | 38.004 | -7.671 | 1.00 | 28.33 |
| 7080 | C | LEU | B | 192 | 30.183 | 39.726 | -5.048 | 1.00 | 26.27 |
| 7081 | O | LEU | B | 192 | 29.890 | 38.580 | -4.737 | 1.00 | 25.80 |
| 7082 | N | ASP | B | 193 | 31.286 | 40.317 | -4.590 | 1.00 | 26.90 |
| 7084 | CA | ASP | B | 193 | 32.198 | 39.558 | -3.721 | 1.00 | 27.11 |
| 7086 | CB | ASP | B | 193 | 33.567 | 40.236 | -3.526 | 1.00 | 27.85 |
| 7089 | CG | ASP | B | 193 | 33.480 | 41.648 | -2.951 | 1.00 | 30.82 |
| 7090 | OD1 | ASP | B | 193 | 34.555 | 42.173 | -2.574 | 1.00 | 36.51 |
| 7091 | OD2 | ASP | B | 193 | 32.435 | 42.331 | -2.848 | 1.00 | 35.53 |
| 7092 | C | ASP | B | 193 | 31.554 | 39.180 | -2.380 | 1.00 | 26.24 |
| 7093 | O | ASP | B | 193 | 31.729 | 38.053 | -1.900 | 1.00 | 25.65 |
| 7094 | N | ALA | B | 194 | 30.809 | 40.117 | -1.799 | 1.00 | 25.42 |
| 7096 | CA | ALA | B | 194 | 30.097 | 39.892 | -0.548 | 1.00 | 24.85 |
| 7098 | CB | ALA | B | 194 | 29.610 | 41.221 | 0.019 | 1.00 | 24.84 |
| 7102 | C | ALA | B | 194 | 28.915 | 38.951 | -0.774 | 1.00 | 24.38 |
| 7103 | O | ALA | B | 194 | 28.578 | 38.154 | 0.081 | 1.00 | 24.14 |
| 7104 | N | LEU | B | 195 | 28.291 | 39.059 | -1.942 | 1.00 | 24.33 |
| 7106 | CA | LEU | B | 195 | 27.156 | 38.230 | -2.286 | 1.00 | 24.42 |
| 7108 | CB | LEU | B | 195 | 26.530 | 38.741 | -3.577 | 1.00 | 24.99 |
| 7111 | CG | LEU | B | 195 | 25.509 | 37.865 | -4.268 | 1.00 | 25.94 |
| 7113 | CD1 | LEU | B | 195 | 24.317 | 37.593 | -3.350 | 1.00 | 26.65 |
| 7117 | CD2 | LEU | B | 195 | 25.072 | 38.566 | -5.566 | 1.00 | 26.30 |
| 7121 | C | LEU | B | 195 | 27.607 | 36.783 | -2.435 | 1.00 | 23.85 |
| 7122 | O | LEU | B | 195 | 26.965 | 35.863 | -1.918 | 1.00 | 23.56 |
| 7123 | N | GLU | B | 196 | 28.727 | 36.590 | -3.115 | 1.00 | 23.22 |
| 7125 | CA | GLU | B | 196 | 29.301 | 35.269 | -3.280 | 1.00 | 23.29 |
| 7127 | CB | GLU | B | 196 | 30.566 | 35.331 | -4.135 | 1.00 | 23.75 |
| 7130 | CG | GLU | B | 196 | 31.070 | 33.963 | -4.535 | 1.00 | 25.63 |
| 7133 | CD | GLU | B | 196 | 32.356 | 33.994 | -5.339 | 1.00 | 28.46 |
| 7134 | OE1 | GLU | B | 196 | 33.201 | 33.121 | -5.090 | 1.00 | 31.64 |
| 7135 | OE2 | GLU | B | 196 | 32.522 | 34.854 | -6.226 | 1.00 | 32.12 |
| 7136 | C | GLU | B | 196 | 29.625 | 34.655 | -1.917 | 1.00 | 22.85 |
| 7137 | O | GLU | B | 196 | 29.434 | 33.459 | -1.699 | 1.00 | 20.62 |
| 7138 | N | ARG | B | 197 | 30.114 | 35.490 | -1.009 | 1.00 | 22.57 |
| 7140 | CA | ARG | B | 197 | 30.499 | 35.041 | 0.315 | 1.00 | 22.97 |
| 7142 | CB | ARG | B | 197 | 31.169 | 36.171 | 1.077 | 1.00 | 23.59 |
| 7145 | CG | ARG | B | 197 | 31.646 | 35.789 | 2.444 | 1.00 | 26.56 |
| 7148 | CD | ARG | B | 197 | 32.707 | 36.714 | 3.004 | 1.00 | 31.42 |
| 7151 | NE | ARG | B | 197 | 32.158 | 37.666 | 3.962 | 1.00 | 35.82 |
| 7153 | CZ | ARG | B | 197 | 32.874 | 38.304 | 4.891 | 1.00 | 38.83 |
| 7154 | NH1 | ARG | B | 197 | 34.184 | 38.105 | 5.012 | 1.00 | 39.90 |
| 7157 | NH2 | ARG | B | 197 | 32.270 | 39.150 | 5.712 | 1.00 | 40.92 |
| 7160 | C | ARG | B | 197 | 29.282 | 34.546 | 1.087 | 1.00 | 21.94 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 7161 | O | ARG | B | 197 | 29.357 | 33.536 | 1.770 | 1.00 | 22.24 |
| 7162 | N | ILE | B | 198 | 28.160 | 35.246 | 0.947 | 1.00 | 21.11 |
| 7164 | CA | ILE | B | 198 | 26.916 | 34.836 | 1.574 | 1.00 | 19.99 |
| 7166 | CB | ILE | B | 198 | 25.763 | 35.775 | 1.186 | 1.00 | 19.92 |
| 7168 | CG1 | ILE | B | 198 | 25.925 | 37.151 | 1.835 | 1.00 | 20.88 |
| 7171 | CD1 | ILE | B | 198 | 25.092 | 38.196 | 1.195 | 1.00 | 21.97 |
| 7175 | CG2 | ILE | B | 198 | 24.408 | 35.196 | 1.598 | 1.00 | 19.49 |
| 7179 | C | ILE | B | 198 | 26.589 | 33.421 | 1.107 | 1.00 | 19.95 |
| 7180 | O | ILE | B | 198 | 26.387 | 32.538 | 1.914 | 1.00 | 19.48 |
| 7181 | N | HIS | B | 199 | 26.542 | 33.231 | -0.207 | 1.00 | 19.56 |
| 7183 | CA | HIS | B | 199 | 26.027 | 31.999 | -0.802 | 1.00 | 18.94 |
| 7185 | CB | HIS | B | 199 | 25.801 | 32.209 | -2.298 | 1.00 | 19.11 |
| 7188 | CG | HIS | B | 199 | 24.584 | 33.024 | -2.606 | 1.00 | 17.67 |
| 7189 | ND1 | HIS | B | 199 | 23.920 | 33.755 | -1.647 | 1.00 | 19.83 |
| 7191 | CE1 | HIS | B | 199 | 22.873 | 34.349 | -2.191 | 1.00 | 19.06 |
| 7193 | NE2 | HIS | B | 199 | 22.821 | 34.013 | -3.467 | 1.00 | 19.16 |
| 7195 | CD2 | HIS | B | 199 | 23.882 | 33.186 | -3.754 | 1.00 | 19.39 |
| 7197 | C | HIS | B | 199 | 26.913 | 30.802 | -0.543 | 1.00 | 18.45 |
| 7198 | O | HIS | B | 199 | 26.422 | 29.700 | -0.294 | 1.00 | 18.16 |
| 7199 | N | ARG | B | 200 | 28.221 | 31.017 | -0.579 | 1.00 | 18.21 |
| 7201 | CA | ARG | B | 200 | 29.157 | 29.954 | -0.301 | 1.00 | 18.14 |
| 7203 | CB | ARG | B | 200 | 30.582 | 30.396 | -0.588 | 1.00 | 18.28 |
| 7206 | CG | ARG | B | 200 | 30.894 | 30.549 | -2.059 | 1.00 | 18.14 |
| 7209 | CD | ARG | B | 200 | 32.368 | 30.534 | -2.332 | 1.00 | 19.86 |
| 7212 | NE | ARG | B | 200 | 32.685 | 30.696 | -3.740 | 1.00 | 20.51 |
| 7214 | CZ | ARG | B | 200 | 32.656 | 29.723 | -4.648 | 1.00 | 23.08 |
| 7215 | NH1 | ARG | B | 200 | 32.326 | 28.482 | -4.320 | 1.00 | 24.68 |
| 7218 | NH2 | ARG | B | 200 | 32.981 | 29.995 | -5.900 | 1.00 | 25.18 |
| 7221 | C | ARG | B | 200 | 29.003 | 29.465 | 1.143 | 1.00 | 18.28 |
| 7222 | O | ARG | B | 200 | 29.037 | 28.267 | 1.392 | 1.00 | 18.15 |
| 7223 | N | HIS | B | 201 | 28.782 | 30.390 | 2.079 | 1.00 | 18.49 |
| 7225 | CA | HIS | B | 201 | 28.558 | 30.036 | 3.479 | 1.00 | 18.76 |
| 7227 | CB | HIS | B | 201 | 28.786 | 31.251 | 4.390 | 1.00 | 18.80 |
| 7230 | CG | HIS | B | 201 | 30.224 | 31.612 | 4.533 | 1.00 | 19.89 |
| 7231 | ND1 | HIS | B | 201 | 30.934 | 32.241 | 3.533 | 1.00 | 21.51 |
| 7233 | CE1 | HIS | B | 201 | 32.186 | 32.408 | 3.925 | 1.00 | 21.57 |
| 7235 | NE2 | HIS | B | 201 | 32.311 | 31.910 | 5.142 | 1.00 | 21.37 |
| 7237 | CD2 | HIS | B | 201 | 31.103 | 31.395 | 5.541 | 1.00 | 21.40 |
| 7239 | C | HIS | B | 201 | 27.170 | 29.430 | 3.697 | 1.00 | 18.88 |
| 7240 | O | HIS | B | 201 | 27.050 | 28.298 | 4.182 | 1.00 | 19.41 |
| 7241 | N | LYS | B | 202 | 26.117 | 30.122 | 3.293 | 1.00 | 18.32 |
| 7243 | CA | LYS | B | 202 | 24.778 | 29.672 | 3.686 | 1.00 | 18.29 |
| 7245 | CB | LYS | B | 202 | 23.725 | 30.764 | 3.506 | 1.00 | 18.11 |
| 7248 | CG | LYS | B | 202 | 23.241 | 31.027 | 2.080 | 1.00 | 17.45 |
| 7251 | CD | LYS | B | 202 | 22.081 | 32.049 | 2.131 | 1.00 | 17.15 |
| 7254 | CE | LYS | B | 202 | 21.634 | 32.547 | 0.768 | 1.00 | 15.61 |
| 7257 | NZ | LYS | B | 202 | 20.235 | 33.122 | 0.794 | 1.00 | 15.01 |
| 7261 | C | LYS | B | 202 | 24.322 | 28.389 | 3.006 | 1.00 | 18.44 |
| 7262 | O | LYS | B | 202 | 23.466 | 27.688 | 3.541 | 1.00 | 18.43 |
| 7263 | N | THR | B | 203 | 24.898 | 28.098 | 1.841 | 1.00 | 17.92 |
| 7265 | CA | THR | B | 203 | 24.454 | 27.009 | 0.983 | 1.00 | 18.22 |
| 7267 | CB | THR | B | 203 | 23.686 | 27.598 | -0.203 | 1.00 | 17.81 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 7269 | OG1 | THR | B | 203 | 22.429 | 28.070 | 0.261 | 1.00 | 18.26 |
| 7271 | CG2 | THR | B | 203 | 23.322 | 26.539 | -1.246 | 1.00 | 18.58 |
| 7275 | C | THR | B | 203 | 25.601 | 26.129 | 0.504 | 1.00 | 17.84 |
| 7276 | O | THR | B | 203 | 25.482 | 24.907 | 0.475 | 1.00 | 18.55 |
| 7277 | N | GLY | B | 204 | 26.703 | 26.746 | 0.104 | 1.00 | 17.60 |
| 7279 | CA | GLY | B | 204 | 27.854 | 26.006 | -0.358 | 1.00 | 17.04 |
| 7282 | C | GLY | B | 204 | 28.469 | 25.112 | 0.708 | 1.00 | 16.72 |
| 7283 | O | GLY | B | 204 | 28.863 | 23.993 | 0.415 | 1.00 | 15.65 |
| 7284 | N | ALA | B | 205 | 28.523 | 25.581 | 1.951 | 1.00 | 16.19 |
| 7286 | CA | ALA | B | 205 | 29.239 | 24.837 | 2.993 | 1.00 | 16.23 |
| 7288 | CB | ALA | B | 205 | 29.265 | 25.611 | 4.271 | 1.00 | 16.00 |
| 7292 | C | ALA | B | 205 | 28.633 | 23.441 | 3.200 | 1.00 | 16.09 |
| 7293 | O | ALA | B | 205 | 29.357 | 22.445 | 3.312 | 1.00 | 16.00 |
| 7294 | N | LEU | B | 206 | 27.309 | 23.363 | 3.200 | 1.00 | 15.80 |
| 7296 | CA | LEU | B | 206 | 26.623 | 22.126 | 3.536 | 1.00 | 16.20 |
| 7298 | CB | LEU | B | 206 | 25.202 | 22.408 | 4.018 | 1.00 | 16.05 |
| 7301 | CG | LEU | B | 206 | 24.363 | 21.238 | 4.540 | 1.00 | 18.16 |
| 7303 | CD1 | LEU | B | 206 | 25.019 | 20.573 | 5.727 | 1.00 | 18.85 |
| 7307 | CD2 | LEU | B | 206 | 22.989 | 21.735 | 4.928 | 1.00 | 18.03 |
| 7311 | C | LEU | B | 206 | 26.593 | 21.206 | 2.332 | 1.00 | 16.19 |
| 7312 | O | LEU | B | 206 | 26.544 | 19.993 | 2.479 | 1.00 | 15.79 |
| 7313 | N | ILE | B | 207 | 26.615 | 21.769 | 1.136 | 1.00 | 16.74 |
| 7315 | CA | ILE | B | 207 | 26.723 | 20.928 | -0.052 | 1.00 | 17.10 |
| 7317 | CB | ILE | B | 207 | 26.341 | 21.713 | -1.305 | 1.00 | 17.41 |
| 7319 | CG1 | ILE | B | 207 | 24.806 | 21.764 | -1.403 | 1.00 | 18.09 |
| 7322 | CD1 | ILE | B | 207 | 24.283 | 22.985 | -2.120 | 1.00 | 19.65 |
| 7326 | CG2 | ILE | B | 207 | 26.936 | 21.073 | -2.581 | 1.00 | 16.41 |
| 7330 | C | ILE | B | 207 | 28.130 | 20.312 | -0.110 | 1.00 | 17.27 |
| 7331 | O | ILE | B | 207 | 28.289 | 19.126 | -0.436 | 1.00 | 16.47 |
| 7332 | N | ARG | B | 208 | 29.139 | 21.098 | 0.240 | 1.00 | 17.03 |
| 7334 | CA | ARG | B | 208 | 30.468 | 20.539 | 0.389 | 1.00 | 17.33 |
| 7336 | CB | ARG | B | 208 | 31.516 | 21.598 | 0.645 | 1.00 | 17.65 |
| 7339 | CG | ARG | B | 208 | 32.956 | 20.997 | 0.625 | 1.00 | 18.08 |
| 7342 | CD | ARG | B | 208 | 34.038 | 22.029 | 0.637 | 1.00 | 19.46 |
| 7345 | NE | ARG | B | 208 | 33.985 | 22.829 | 1.854 | 1.00 | 21.33 |
| 7347 | CZ | ARG | B | 208 | 34.772 | 23.882 | 2.089 | 1.00 | 22.51 |
| 7348 | NH1 | ARG | B | 208 | 34.662 | 24.547 | 3.222 | 1.00 | 23.90 |
| 7351 | NH2 | ARG | B | 208 | 35.663 | 24.271 | 1.199 | 1.00 | 21.54 |
| 7354 | C | ARG | B | 208 | 30.517 | 19.475 | 1.475 | 1.00 | 17.44 |
| 7355 | O | ARG | B | 208 | 31.179 | 18.451 | 1.295 | 1.00 | 17.53 |
| 7356 | N | ALA | B | 209 | 29.804 | 19.689 | 2.580 | 1.00 | 17.13 |
| 7358 | CA | ALA | B | 209 | 29.776 | 18.709 | 3.658 | 1.00 | 16.93 |
| 7360 | CB | ALA | B | 209 | 28.967 | 19.200 | 4.832 | 1.00 | 17.56 |
| 7364 | C | ALA | B | 209 | 29.211 | 17.389 | 3.179 | 1.00 | 17.03 |
| 7365 | O | ALA | B | 209 | 29.704 | 16.351 | 3.574 | 1.00 | 15.70 |
| 7366 | N | ALA | B | 210 | 28.154 | 17.439 | 2.368 | 1.00 | 16.79 |
| 7368 | CA | ALA | B | 210 | 27.548 | 16.224 | 1.799 | 1.00 | 17.41 |
| 7370 | CB | ALA | B | 210 | 26.386 | 16.572 | 0.915 | 1.00 | 17.51 |
| 7374 | C | ALA | B | 210 | 28.560 | 15.419 | 1.002 | 1.00 | 17.70 |
| 7375 | O | ALA | B | 210 | 28.698 | 14.197 | 1.200 | 1.00 | 17.88 |
| 7376 | N | VAL | B | 211 | 29.268 | 16.107 | 0.109 | 1.00 | 17.07 |
| 7378 | CA | VAL | B | 211 | 30.282 | 15.471 | -0.724 | 1.00 | 17.54 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 7380 | CB | VAL | B | 211 | 30.849 | 16.429 | -1.793 | 1.00 | 17.01 |
| 7382 | CG1 | VAL | B | 211 | 31.962 | 15.769 | -2.607 | 1.00 | 17.61 |
| 7386 | CG2 | VAL | B | 211 | 29.750 | 16.884 | -2.730 | 1.00 | 17.80 |
| 7390 | C | VAL | B | 211 | 31.400 | 14.924 | 0.150 | 1.00 | 18.04 |
| 7391 | O | VAL | B | 211 | 31.802 | 13.766 | -0.005 | 1.00 | 17.71 |
| 7392 | N | ARG | B | 212 | 31.887 | 15.748 | 1.078 | 1.00 | 18.26 |
| 7394 | CA | ARG | B | 212 | 32.974 | 15.348 | 1.963 | 1.00 | 18.54 |
| 7396 | CB | ARG | B | 212 | 33.393 | 16.497 | 2.878 | 1.00 | 19.04 |
| 7399 | CG | ARG | B | 212 | 34.211 | 17.532 | 2.179 | 1.00 | 18.96 |
| 7402 | CD | ARG | B | 212 | 34.665 | 18.637 | 3.113 | 1.00 | 20.46 |
| 7405 | NE | ARG | B | 212 | 35.712 | 19.448 | 2.531 | 1.00 | 20.99 |
| 7407 | CZ | ARG | B | 212 | 36.218 | 20.545 | 3.102 | 1.00 | 21.01 |
| 7408 | NH1 | ARG | B | 212 | 35.771 | 20.974 | 4.275 | 1.00 | 20.38 |
| 7411 | NH2 | ARG | B | 212 | 37.190 | 21.204 | 2.495 | 1.00 | 20.62 |
| 7414 | C | ARG | B | 212 | 32.582 | 14.152 | 2.795 | 1.00 | 18.87 |
| 7415 | O | ARG | B | 212 | 33.368 | 13.219 | 2.935 | 1.00 | 18.67 |
| 7416 | N | LEU | B | 213 | 31.346 | 14.136 | 3.289 | 1.00 | 19.33 |
| 7418 | CA | LEU | B | 213 | 30.896 | 13.036 | 4.141 | 1.00 | 20.12 |
| 7420 | CB | LEU | B | 213 | 29.516 | 13.310 | 4.738 | 1.00 | 19.99 |
| 7423 | CG | LEU | B | 213 | 29.431 | 13.776 | 6.203 | 1.00 | 22.44 |
| 7425 | CD1 | LEU | B | 213 | 30.464 | 14.770 | 6.559 | 1.00 | 24.69 |
| 7429 | CD2 | LEU | B | 213 | 28.046 | 14.364 | 6.440 | 1.00 | 24.61 |
| 7433 | C | LEU | B | 213 | 30.887 | 11.715 | 3.370 | 1.00 | 20.21 |
| 7434 | O | LEU | B | 213 | 31.247 | 10.668 | 3.922 | 1.00 | 20.74 |
| 7435 | N | GLY | B | 214 | 30.461 | 11.750 | 2.110 | 1.00 | 20.90 |
| 7437 | CA | GLY | B | 214 | 30.546 | 10.578 | 1.246 | 1.00 | 21.11 |
| 7440 | C | GLY | B | 214 | 31.979 | 10.097 | 1.066 | 1.00 | 21.83 |
| 7441 | O | GLY | B | 214 | 32.263 | 8.898 | 1.152 | 1.00 | 22.91 |
| 7442 | N | ALA | B | 215 | 32.892 | 11.029 | 0.821 | 1.00 | 21.98 |
| 7444 | CA | ALA | B | 215 | 34.292 | 10.688 | 0.627 | 1.00 | 22.48 |
| 7446 | CB | ALA | B | 215 | 35.059 | 11.868 | 0.052 | 1.00 | 22.44 |
| 7450 | C | ALA | B | 215 | 34.934 | 10.189 | 1.928 | 1.00 | 23.19 |
| 7451 | O | ALA | B | 215 | 35.703 | 9.232 | 1.906 | 1.00 | 23.21 |
| 7452 | N | LEU | B | 216 | 34.582 | 10.804 | 3.058 | 1.00 | 23.38 |
| 7454 | CA | LEU | B | 216 | 35.144 | 10.429 | 4.355 | 1.00 | 23.77 |
| 7456 | CB | LEU | B | 216 | 34.733 | 11.429 | 5.440 | 1.00 | 23.69 |
| 7459 | CG | LEU | B | 216 | 35.459 | 12.768 | 5.355 | 1.00 | 23.52 |
| 7461 | CD1 | LEU | B | 216 | 34.830 | 13.745 | 6.336 | 1.00 | 22.14 |
| 7465 | CD2 | LEU | B | 216 | 36.962 | 12.569 | 5.630 | 1.00 | 24.32 |
| 7469 | C | LEU | B | 216 | 34.721 | 9.031 | 4.780 | 1.00 | 24.42 |
| 7470 | O | LEU | B | 216 | 35.379 | 8.410 | 5.603 | 1.00 | 24.38 |
| 7471 | N | SER | B | 217 | 33.627 | 8.541 | 4.211 | 1.00 | 25.75 |
| 7473 | CA | SER | B | 217 | 33.176 | 7.180 | 4.458 | 1.00 | 26.29 |
| 7475 | CB | BSER | B | 217 | 31.724 | 6.990 | 3.992 | 0.35 | 26.33 |
| 7476 | CB | ASER | B | 217 | 31.733 | 7.003 | 3.960 | 0.65 | 26.73 |
| 7481 | OG | BSER | B | 217 | 31.635 | 6.814 | 2.589 | 0.35 | 25.17 |
| 7482 | OG | ASER | B | 217 | 30.884 | 8.043 | 4.437 | 0.65 | 28.22 |
| 7485 | C | SER | B | 217 | 34.096 | 6.146 | 3.779 | 1.00 | 26.79 |
| 7486 | O | SER | B | 217 | 33.943 | 4.960 | 4.011 | 1.00 | 27.11 |
| 7487 | N | ALA | B | 218 | 35.052 | 6.609 | 2.971 | 1.00 | 27.48 |
| 7489 | CA | ALA | B | 218 | 35.807 | 5.765 | 2.045 | 1.00 | 28.00 |
| 7491 | CB | ALA | B | 218 | 35.502 | 6.200 | 0.610 | 1.00 | 27.64 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 7495 | C | ALA | B | 218 | 37.330 | 5.735 | 2.259 | 1.00 | 28.36 |
| 7496 | O | ALA | B | 218 | 38.075 | 5.478 | 1.305 | 1.00 | 28.63 |
| 7497 | N | GLY | B | 219 | 37.793 | 6.017 | 3.480 | 1.00 | 28.63 |
| 7499 | CA | GLY | B | 219 | 39.190 | 5.812 | 3.848 | 1.00 | 28.66 |
| 7502 | C | GLY | B | 219 | 40.160 | 6.623 | 3.013 | 1.00 | 29.30 |
| 7503 | O | GLY | B | 219 | 39.829 | 7.754 | 2.628 | 1.00 | 29.18 |
| 7504 | N | ASP | B | 220 | 41.337 | 6.047 | 2.725 | 1.00 | 29.91 |
| 7506 | CA | ASP | B | 220 | 42.401 | 6.716 | 1.945 | 1.00 | 30.40 |
| 7508 | CB | ASP | B | 220 | 43.629 | 5.798 | 1.749 | 1.00 | 31.13 |
| 7511 | CG | ASP | B | 220 | 44.248 | 5.315 | 3.055 | 1.00 | 32.74 |
| 7512 | OD1 | ASP | B | 220 | 44.060 | 5.963 | 4.113 | 1.00 | 34.47 |
| 7513 | OD2 | ASP | B | 220 | 44.958 | 4.280 | 3.097 | 1.00 | 35.20 |
| 7514 | C | ASP | B | 220 | 41.960 | 7.157 | 0.541 | 1.00 | 30.05 |
| 7515 | O | ASP | B | 220 | 42.333 | 8.224 | 0.068 | 1.00 | 29.72 |
| 7516 | N | LYS | B | 221 | 41.203 | 6.319 | -0.150 | 1.00 | 30.05 |
| 7518 | CA | LYS | B | 221 | 40.854 | 6.614 | -1.546 | 1.00 | 29.92 |
| 7520 | CB | LYS | B | 221 | 40.230 | 5.391 | -2.199 | 1.00 | 30.71 |
| 7523 | CG | LYS | B | 221 | 40.214 | 5.394 | -3.723 | 1.00 | 32.45 |
| 7526 | CD | LYS | B | 221 | 39.887 | 3.980 | -4.222 | 1.00 | 34.64 |
| 7529 | CE | LYS | B | 221 | 39.790 | 3.882 | -5.732 | 1.00 | 36.80 |
| 7532 | NZ | LYS | B | 221 | 39.315 | 2.521 | -6.190 | 1.00 | 38.07 |
| 7536 | C | LYS | B | 221 | 39.906 | 7.821 | -1.634 | 1.00 | 28.89 |
| 7537 | O | LYS | B | 221 | 40.045 | 8.661 | -2.525 | 1.00 | 28.45 |
| 7538 | N | GLY | B | 222 | 38.972 | 7.902 | -0.689 | 1.00 | 27.81 |
| 7540 | CA | GLY | B | 222 | 38.049 | 9.018 | -0.591 | 1.00 | 27.11 |
| 7543 | C | GLY | B | 222 | 38.781 | 10.292 | -0.243 | 1.00 | 26.53 |
| 7544 | O | GLY | B | 222 | 38.559 | 11.333 | -0.840 | 1.00 | 26.52 |
| 7545 | N | ARG | B | 223 | 39.690 | 10.198 | 0.720 | 1.00 | 26.28 |
| 7547 | CA | ARG | B | 223 | 40.519 | 11.340 | 1.099 | 1.00 | 25.74 |
| 7549 | CB | ARG | B | 223 | 41.263 | 11.018 | 2.393 | 1.00 | 25.35 |
| 7552 | CG | ARG | B | 223 | 40.332 | 11.005 | 3.598 | 1.00 | 28.38 |
| 7555 | CD | ARG | B | 223 | 40.945 | 10.453 | 4.857 | 1.00 | 31.47 |
| 7558 | NE | ARG | B | 223 | 40.208 | 10.787 | 6.078 | 1.00 | 33.37 |
| 7560 | CZ | ARG | B | 223 | 40.258 | 11.974 | 6.697 | 1.00 | 36.00 |
| 7561 | NH1 | ARG | B | 223 | 40.977 | 12.979 | 6.200 | 1.00 | 39.28 |
| 7564 | NH2 | ARG | B | 223 | 39.575 | 12.170 | 7.810 | 1.00 | 34.96 |
| 7567 | C | ARG | B | 223 | 41.471 | 11.800 | -0.027 | 1.00 | 24.69 |
| 7568 | O | ARG | B | 223 | 41.743 | 12.983 | -0.161 | 1.00 | 24.52 |
| 7569 | N | ARG | B | 224 | 41.956 | 10.873 | -0.844 | 1.00 | 24.21 |
| 7571 | CA | ARG | B | 224 | 42.809 | 11.210 | -1.983 | 1.00 | 23.79 |
| 7573 | CB | ARG | B | 224 | 43.340 | 9.927 | -2.637 | 1.00 | 24.37 |
| 7576 | CG | ARG | B | 224 | 44.257 | 10.097 | -3.872 | 1.00 | 27.47 |
| 7579 | CD | ARG | B | 224 | 43.908 | 9.115 | -5.003 | 1.00 | 32.66 |
| 7582 | NE | ARG | B | 224 | 45.013 | 8.799 | -5.908 | 1.00 | 36.58 |
| 7584 | CZ | ARG | B | 224 | 45.406 | 9.552 | -6.933 | 1.00 | 39.40 |
| 7585 | NH1 | ARG | B | 224 | 46.425 | 9.145 | -7.688 | 1.00 | 40.57 |
| 7588 | NH2 | ARG | B | 224 | 44.809 | 10.714 | -7.204 | 1.00 | 39.74 |
| 7591 | C | ARG | B | 224 | 42.025 | 12.047 | -3.005 | 1.00 | 22.91 |
| 7592 | O | ARG | B | 224 | 42.599 | 12.928 | -3.640 | 1.00 | 22.18 |
| 7593 | N | ALA | B | 225 | 40.726 | 11.759 | -3.149 | 1.00 | 21.70 |
| 7595 | CA | ALA | B | 225 | 39.845 | 12.476 | -4.066 | 1.00 | 21.49 |
| 7597 | CB | ALA | B | 225 | 38.667 | 11.618 | -4.422 | 1.00 | 21.35 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 7601 | C | ALA | B | 225 | 39.340 | 13.818 | -3.523 | 1.00 | 21.64 |
| 7602 | O | ALA | B | 225 | 38.756 | 14.587 | -4.270 | 1.00 | 20.84 |
| 7603 | N | LEU | B | 226 | 39.563 | 14.090 | -2.240 | 1.00 | 21.58 |
| 7605 | CA | LEU | B | 226 | 39.003 | 15.285 | -1.600 | 1.00 | 22.20 |
| 7607 | CB | LEU | B | 226 | 39.340 | 15.335 | -0.110 | 1.00 | 22.43 |
| 7610 | CG | LEU | B | 226 | 38.407 | 14.580 | 0.840 | 1.00 | 22.95 |
| 7612 | CD1 | LEU | B | 226 | 38.991 | 14.642 | 2.244 | 1.00 | 24.14 |
| 7616 | CD2 | LEU | B | 226 | 37.002 | 15.153 | 0.810 | 1.00 | 24.62 |
| 7620 | C | LEU | B | 226 | 39.364 | 16.616 | -2.239 | 1.00 | 21.85 |
| 7621 | O | LEU | B | 226 | 38.482 | 17.438 | -2.393 | 1.00 | 22.54 |
| 7622 | N | PRO | B | 227 | 40.627 | 16.872 | -2.583 | 1.00 | 22.19 |
| 7623 | CA | PRO | B | 227 | 40.969 | 18.150 | -3.227 | 1.00 | 22.28 |
| 7625 | CB | PRO | B | 227 | 42.442 | 17.987 | -3.589 | 1.00 | 22.39 |
| 7628 | CG | PRO | B | 227 | 42.951 | 16.960 | -2.616 | 1.00 | 23.34 |
| 7631 | CD | PRO | B | 227 | 41.812 | 16.025 | -2.379 | 1.00 | 22.27 |
| 7634 | C | PRO | B | 227 | 40.115 | 18.420 | -4.460 | 1.00 | 21.79 |
| 7635 | O | PRO | B | 227 | 39.580 | 19.513 | -4.592 | 1.00 | 21.54 |
| 7636 | N | VAL | B | 228 | 39.945 | 17.431 | -5.331 | 1.00 | 21.34 |
| 7638 | CA | VAL | B | 228 | 39.131 | 17.616 | -6.533 | 1.00 | 20.96 |
| 7640 | CB | VAL | B | 228 | 39.431 | 16.533 | -7.601 | 1.00 | 21.09 |
| 7642 | CG1 | VAL | B | 228 | 38.492 | 16.664 | -8.787 | 1.00 | 20.79 |
| 7646 | CG2 | VAL | B | 228 | 40.885 | 16.668 | -8.085 | 1.00 | 22.50 |
| 7650 | C | VAL | B | 228 | 37.620 | 17.635 | -6.214 | 1.00 | 20.48 |
| 7651 | O | VAL | B | 228 | 36.877 | 18.411 | -6.804 | 1.00 | 20.29 |
| 7652 | N | LEU | B | 229 | 37.172 | 16.773 | -5.307 | 1.00 | 20.17 |
| 7654 | CA | LEU | B | 229 | 35.750 | 16.717 | -4.924 | 1.00 | 19.91 |
| 7656 | CB | LEU | B | 229 | 35.466 | 15.562 | -3.957 | 1.00 | 20.52 |
| 7659 | CG | LEU | B | 229 | 35.293 | 14.173 | -4.587 | 1.00 | 21.95 |
| 7661 | CD1 | LEU | B | 229 | 35.296 | 13.095 | -3.512 | 1.00 | 22.04 |
| 7665 | CD2 | LEU | B | 229 | 34.039 | 14.111 | -5.407 | 1.00 | 23.07 |
| 7669 | C | LEU | B | 229 | 35.327 | 18.015 | -4.253 | 1.00 | 19.72 |
| 7670 | O | LEU | B | 229 | 34.188 | 18.456 | -4.381 | 1.00 | 19.07 |
| 7671 | N | ASP | B | 230 | 36.250 | 18.599 | -3.503 | 1.00 | 19.68 |
| 7673 | CA | ASP | B | 230 | 36.042 | 19.893 | -2.883 | 1.00 | 19.94 |
| 7675 | CB | ASP | B | 230 | 37.272 | 20.287 | -2.069 | 1.00 | 19.86 |
| 7678 | CG | ASP | B | 230 | 37.289 | 19.671 | -0.705 | 1.00 | 22.67 |
| 7679 | OD1 | ASP | B | 230 | 36.256 | 19.094 | -0.288 | 1.00 | 23.35 |
| 7680 | OD2 | ASP | B | 230 | 38.304 | 19.744 | 0.036 | 1.00 | 25.14 |
| 7681 | C | ASP | B | 230 | 35.778 | 20.972 | -3.908 | 1.00 | 19.81 |
| 7682 | O | ASP | B | 230 | 34.910 | 21.795 | -3.702 | 1.00 | 19.95 |
| 7683 | N | LYS | B | 231 | 36.541 | 20.990 | -4.996 | 1.00 | 19.94 |
| 7685 | CA | LYS | B | 231 | 36.368 | 22.027 | -6.013 | 1.00 | 20.31 |
| 7687 | CB | LYS | B | 231 | 37.525 | 22.048 | -7.022 | 1.00 | 20.63 |
| 7690 | CG | LYS | B | 231 | 38.973 | 22.184 | -6.439 | 1.00 | 22.72 |
| 7693 | CD | BLYS | B | 231 | 39.100 | 23.053 | -5.155 | 0.35 | 21.46 |
| 7694 | CD | ALYS | B | 231 | 39.001 | 22.753 | -5.014 | 0.65 | 25.09 |
| 7699 | CE | BLYS | B | 231 | 39.223 | 22.270 | -3.837 | 0.35 | 19.92 |
| 7700 | CE | ALYS | B | 231 | 39.871 | 23.974 | -4.801 | 0.65 | 25.51 |
| 7705 | NZ | BLYS | B | 231 | 40.570 | 21.728 | -3.502 | 0.35 | 14.63 |
| 7706 | NZ | ALYS | B | 231 | 39.377 | 24.575 | -3.546 | 0.65 | 24.29 |
| 7713 | C | LYS | B | 231 | 35.049 | 21.804 | -6.718 | 1.00 | 19.81 |
| 7714 | O | LYS | B | 231 | 34.320 | 22.762 | -6.982 | 1.00 | 19.64 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 7715 | N | TYR | B | 232 | 34.733 | 20.536 | -6.979 | 1.00 | 19.10 |
| 7717 | CA | TYR | B | 232 | 33.437 | 20.151 | -7.525 | 1.00 | 18.47 |
| 7719 | CB | TYR | B | 232 | 33.307 | 18.624 | -7.646 | 1.00 | 18.62 |
| 7722 | CG | TYR | B | 232 | 31.883 | 18.168 | -7.875 | 1.00 | 17.81 |
| 7723 | CD1 | TYR | B | 232 | 31.300 | 18.256 | -9.132 | 1.00 | 17.52 |
| 7725 | CE1 | TYR | B | 232 | 29.994 | 17.859 | -9.337 | 1.00 | 20.05 |
| 7727 | CZ | TYR | B | 232 | 29.232 | 17.374 | -8.279 | 1.00 | 18.47 |
| 7728 | OH | TYR | B | 232 | 27.919 | 16.982 | -8.500 | 1.00 | 17.52 |
| 7730 | CE2 | TYR | B | 232 | 29.785 | 17.299 | -7.026 | 1.00 | 17.57 |
| 7732 | CD2 | TYR | B | 232 | 31.112 | 17.694 | -6.829 | 1.00 | 17.49 |
| 7734 | C | TYR | B | 232 | 32.331 | 20.699 | -6.643 | 1.00 | 18.41 |
| 7735 | O | TYR | B | 232 | 31.452 | 21.411 | -7.122 | 1.00 | 18.11 |
| 7736 | N | ALA | B | 233 | 32.417 | 20.408 | -5.345 | 1.00 | 18.13 |
| 7738 | CA | ALA | B | 233 | 31.403 | 20.799 | -4.377 | 1.00 | 18.18 |
| 7740 | CB | ALA | B | 233 | 31.723 | 20.221 | -3.021 | 1.00 | 17.94 |
| 7744 | C | ALA | B | 233 | 31.281 | 22.316 | -4.251 | 1.00 | 18.61 |
| 7745 | O | ALA | B | 233 | 30.196 | 22.851 | -4.063 | 1.00 | 18.11 |
| 7746 | N | GLU | B | 234 | 32.407 | 22.996 | -4.328 | 1.00 | 19.06 |
| 7748 | CA | GLU | B | 234 | 32.418 | 24.439 | -4.177 | 1.00 | 20.24 |
| 7750 | CB | GLU | B | 234 | 33.864 | 24.949 | -4.123 | 1.00 | 20.64 |
| 7753 | CG | GLU | B | 234 | 34.451 | 24.809 | -2.730 | 1.00 | 23.29 |
| 7756 | CD | GLU | B | 234 | 35.947 | 24.586 | -2.731 | 1.00 | 26.70 |
| 7757 | OE1 | GLU | B | 234 | 36.464 | 23.942 | -1.768 | 1.00 | 29.92 |
| 7758 | OE2 | GLU | B | 234 | 36.592 | 25.044 | -3.686 | 1.00 | 27.85 |
| 7759 | C | GLU | B | 234 | 31.636 | 25.080 | -5.300 | 1.00 | 20.03 |
| 7760 | O | GLU | B | 234 | 30.842 | 25.982 | -5.063 | 1.00 | 20.42 |
| 7761 | N | SER | B | 235 | 31.824 | 24.584 | -6.521 | 1.00 | 20.10 |
| 7763 | CA | SER | B | 235 | 31.140 | 25.146 | -7.663 | 1.00 | 20.21 |
| 7765 | CB | SER | B | 235 | 31.838 | 24.755 | -8.958 | 1.00 | 20.74 |
| 7768 | OG | SER | B | 235 | 33.134 | 25.319 | -8.986 | 1.00 | 21.81 |
| 7770 | C | SER | B | 235 | 29.655 | 24.795 | -7.704 | 1.00 | 19.69 |
| 7771 | O | SER | B | 235 | 28.845 | 25.675 | -7.972 | 1.00 | 19.58 |
| 7772 | N | ILE | B | 236 | 29.283 | 23.538 | -7.451 | 1.00 | 19.26 |
| 7774 | CA | ILE | B | 236 | 27.855 | 23.173 | -7.467 | 1.00 | 19.00 |
| 7776 | CB | ILE | B | 236 | 27.588 | 21.634 | -7.493 | 1.00 | 19.39 |
| 7778 | CG1 | ILE | B | 236 | 28.132 | 20.922 | -6.249 | 1.00 | 19.42 |
| 7781 | CD1 | ILE | B | 236 | 27.348 | 19.661 | -5.883 | 1.00 | 19.21 |
| 7785 | CG2 | ILE | B | 236 | 28.145 | 20.996 | -8.778 | 1.00 | 20.74 |
| 7789 | C | ILE | B | 236 | 27.118 | 23.798 | -6.292 | 1.00 | 18.75 |
| 7790 | O | ILE | B | 236 | 25.934 | 24.062 | -6.404 | 1.00 | 18.69 |
| 7791 | N | GLY | B | 237 | 27.825 | 24.000 | -5.179 | 1.00 | 17.92 |
| 7793 | CA | GLY | B | 237 | 27.260 | 24.588 | -3.977 | 1.00 | 18.54 |
| 7796 | C | GLY | B | 237 | 26.885 | 26.044 | -4.189 | 1.00 | 18.41 |
| 7797 | O | GLY | B | 237 | 25.776 | 26.467 | -3.838 | 1.00 | 18.39 |
| 7798 | N | LEU | B | 238 | 27.791 | 26.809 | -4.801 | 1.00 | 18.03 |
| 7800 | CA | LEU | B | 238 | 27.463 | 28.191 | -5.176 | 1.00 | 17.92 |
| 7802 | CB | LEU | B | 238 | 28.697 | 28.973 | -5.644 | 1.00 | 17.76 |
| 7805 | CG | LEU | B | 238 | 28.471 | 30.416 | -6.137 | 1.00 | 18.58 |
| 7807 | CD1 | LEU | B | 238 | 27.676 | 31.245 | -5.123 | 1.00 | 20.10 |
| 7811 | CD2 | LEU | B | 238 | 29.783 | 31.085 | -6.471 | 1.00 | 19.77 |
| 7815 | C | LEU | B | 238 | 26.371 | 28.184 | -6.232 | 1.00 | 17.69 |
| 7816 | O | LEU | B | 238 | 25.391 | 28.929 | -6.125 | 1.00 | 17.69 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 7817 | N | ALA | B | 239 | 26.520 | 27.332 | -7.243 | 1.00 | 17.54 |
| 7819 | CA | ALA | B | 239 | 25.535 | 27.255 | -8.330 | 1.00 | 17.52 |
| 7821 | CB | ALA | B | 239 | 25.937 | 26.175 | -9.322 | 1.00 | 17.72 |
| 7825 | C | ALA | B | 239 | 24.133 | 26.996 | -7.801 | 1.00 | 16.87 |
| 7826 | O | ALA | B | 239 | 23.149 | 27.503 | -8.321 | 1.00 | 16.72 |
| 7827 | N | PHE | B | 240 | 24.055 | 26.207 | -6.738 | 1.00 | 17.20 |
| 7829 | CA | PHE | B | 240 | 22.796 | 25.770 | -6.175 | 1.00 | 17.20 |
| 7831 | CB | PHE | B | 240 | 23.077 | 24.798 | -5.020 | 1.00 | 17.86 |
| 7834 | CG | PHE | B | 240 | 21.913 | 23.952 | -4.635 | 1.00 | 19.19 |
| 7835 | CD1 | PHE | B | 240 | 21.908 | 22.595 | -4.939 | 1.00 | 23.96 |
| 7837 | CE1 | PHE | B | 240 | 20.833 | 21.786 | -4.576 | 1.00 | 25.08 |
| 7839 | CZ | PHE | B | 240 | 19.753 | 22.346 | -3.895 | 1.00 | 23.44 |
| 7841 | CE2 | PHE | B | 240 | 19.766 | 23.705 | -3.578 | 1.00 | 21.13 |
| 7843 | CD2 | PHE | B | 240 | 20.837 | 24.489 | -3.936 | 1.00 | 19.81 |
| 7845 | C | PHE | B | 240 | 22.023 | 26.972 | -5.659 | 1.00 | 17.12 |
| 7846 | O | PHE | B | 240 | 20.817 | 27.075 | -5.856 | 1.00 | 16.09 |
| 7847 | N | GLN | B | 241 | 22.724 | 27.860 | -4.969 | 1.00 | 16.71 |
| 7849 | CA | GLN | B | 241 | 22.093 | 29.040 | -4.427 | 1.00 | 17.18 |
| 7851 | CB | GLN | B | 241 | 22.918 | 29.661 | -3.304 | 1.00 | 16.88 |
| 7854 | CG | GLN | B | 241 | 22.173 | 30.781 | -2.566 | 1.00 | 16.78 |
| 7857 | CD | GLN | B | 241 | 20.856 | 30.332 | -1.970 | 1.00 | 18.18 |
| 7858 | OE1 | GLN | B | 241 | 20.783 | 29.271 | -1.353 | 1.00 | 17.96 |
| 7859 | NE2 | GLN | B | 241 | 19.818 | 31.140 | -2.138 | 1.00 | 15.32 |
| 7862 | C | GLN | B | 241 | 21.821 | 30.089 | -5.501 | 1.00 | 16.98 |
| 7863 | O | GLN | B | 241 | 20.842 | 30.800 | -5.392 | 1.00 | 16.15 |
| 7864 | N | VAL | B | 242 | 22.640 | 30.184 | -6.544 | 1.00 | 17.46 |
| 7866 | CA | VAL | B | 242 | 22.265 | 31.160 | -7.590 | 1.00 | 18.23 |
| 7868 | CB | VAL | B | 242 | 23.405 | 31.708 | -8.547 | 1.00 | 18.68 |
| 7870 | CG1 | VAL | B | 242 | 24.747 | 31.119 | -8.271 | 1.00 | 19.87 |
| 7874 | CG2 | VAL | B | 242 | 23.019 | 31.733 | -10.030 | 1.00 | 19.70 |
| 7878 | C | VAL | B | 242 | 21.003 | 30.665 | -8.279 | 1.00 | 17.45 |
| 7879 | O | VAL | B | 242 | 20.139 | 31.457 | -8.531 | 1.00 | 17.04 |
| 7880 | N | GLN | B | 243 | 20.856 | 29.350 | -8.447 | 1.00 | 17.88 |
| 7882 | CA | GLN | B | 243 | 19.649 | 28.785 | -9.035 | 1.00 | 18.28 |
| 7884 | CB | GLN | B | 243 | 19.783 | 27.288 | -9.337 | 1.00 | 18.86 |
| 7887 | CG | GLN | B | 243 | 18.561 | 26.715 | -10.056 | 1.00 | 20.61 |
| 7890 | CD | GLN | B | 243 | 18.402 | 27.211 | -11.478 | 1.00 | 23.91 |
| 7891 | OE1 | GLN | B | 243 | 19.207 | 27.995 | -11.962 | 1.00 | 27.71 |
| 7892 | NE2 | GLN | B | 243 | 17.361 | 26.738 | -12.157 | 1.00 | 25.53 |
| 7895 | C | GLN | B | 243 | 18.469 | 29.005 | -8.135 | 1.00 | 17.68 |
| 7896 | O | GLN | B | 243 | 17.381 | 29.326 | -8.612 | 1.00 | 18.18 |
| 7897 | N | ASP | B | 244 | 18.673 | 28.830 | -6.832 | 1.00 | 16.95 |
| 7899 | CA | ASP | B | 244 | 17.624 | 29.133 | -5.872 | 1.00 | 16.59 |
| 7901 | CB | ASP | B | 244 | 18.084 | 28.803 | -4.452 | 1.00 | 15.86 |
| 7904 | CG | ASP | B | 244 | 16.988 | 28.976 | -3.451 | 1.00 | 16.32 |
| 7905 | OD1 | ASP | B | 244 | 16.037 | 28.162 | -3.445 | 1.00 | 17.49 |
| 7906 | OD2 | ASP | B | 244 | 16.959 | 29.929 | -2.651 | 1.00 | 18.97 |
| 7907 | C | ASP | B | 244 | 17.186 | 30.610 | -5.985 | 1.00 | 16.34 |
| 7908 | O | ASP | B | 244 | 16.001 | 30.905 | -5.932 | 1.00 | 15.59 |
| 7909 | N | ASP | B | 245 | 18.135 | 31.526 | -6.146 | 1.00 | 17.76 |
| 7911 | CA | ASP | B | 245 | 17.799 | 32.959 | -6.321 | 1.00 | 18.83 |
| 7913 | CB | ASP | B | 245 | 19.044 | 33.819 | -6.384 | 1.00 | 19.28 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 7916 | CG | ASP | B | 245 | 19.766 | 33.928 | -5.070 | 1.00 | 19.95 |
| 7917 | OD1 | ASP | B | 245 | 19.251 | 33.447 | -4.018 | 1.00 | 23.46 |
| 7918 | OD2 | ASP | B | 245 | 20.886 | 34.480 | -5.016 | 1.00 | 19.63 |
| 7919 | C | ASP | B | 245 | 17.021 | 33.192 | -7.610 | 1.00 | 19.87 |
| 7920 | O | ASP | B | 245 | 16.020 | 33.917 | -7.629 | 1.00 | 20.25 |
| 7921 | N | ILE | B | 246 | 17.492 | 32.570 | -8.687 | 1.00 | 19.96 |
| 7923 | CA | ILE | B | 246 | 16.845 | 32.676 | -9.986 | 1.00 | 20.61 |
| 7925 | CB | ILE | B | 246 | 17.647 | 31.902 | -11.039 | 1.00 | 20.77 |
| 7927 | CG1 | ILE | B | 246 | 18.945 | 32.645 | -11.363 | 1.00 | 20.81 |
| 7930 | CD1 | ILE | B | 246 | 19.974 | 31.792 | -11.997 | 1.00 | 21.71 |
| 7934 | CG2 | ILE | B | 246 | 16.821 | 31.682 | -12.304 | 1.00 | 21.31 |
| 7938 | C | ILE | B | 246 | 15.413 | 32.161 | -9.932 | 1.00 | 20.80 |
| 7939 | O | ILE | B | 246 | 14.506 | 32.784 | -10.482 | 1.00 | 20.05 |
| 7940 | N | LEU | B | 247 | 15.214 | 31.014 | -9.283 | 1.00 | 21.23 |
| 7942 | CA | LEU | B | 247 | 13.904 | 30.394 | -9.206 | 1.00 | 21.82 |
| 7944 | CB | LEU | B | 247 | 14.009 | 28.986 | -8.620 | 1.00 | 22.08 |
| 7947 | CG | LEU | B | 247 | 14.569 | 27.953 | -9.600 | 1.00 | 23.04 |
| 7949 | CD1 | LEU | B | 247 | 14.635 | 26.592 | -8.926 | 1.00 | 25.03 |
| 7953 | CD2 | LEU | B | 247 | 13.740 | 27.874 | -10.869 | 1.00 | 23.91 |
| 7957 | C | LEU | B | 247 | 12.955 | 31.226 | -8.384 | 1.00 | 22.17 |
| 7958 | O | LEU | B | 247 | 11.759 | 31.219 | -8.613 | 1.00 | 22.86 |
| 7959 | N | ASP | B | 248 | 13.487 | 31.928 | -7.401 | 1.00 | 22.89 |
| 7961 | CA | ASP | B | 248 | 12.680 | 32.816 | -6.597 | 1.00 | 23.68 |
| 7963 | CB | ASP | B | 248 | 13.538 | 33.476 | -5.526 | 1.00 | 24.26 |
| 7966 | CG | ASP | B | 248 | 12.782 | 33.732 | -4.261 | 1.00 | 26.59 |
| 7967 | OD1 | ASP | B | 248 | 12.339 | 34.885 | -4.081 | 1.00 | 29.09 |
| 7968 | OD2 | ASP | B | 248 | 12.586 | 32.842 | -3.395 | 1.00 | 30.35 |
| 7969 | C | ASP | B | 248 | 12.018 | 33.889 | -7.468 | 1.00 | 24.03 |
| 7970 | O | ASP | B | 248 | 10.872 | 34.264 | -7.225 | 1.00 | 23.75 |
| 7971 | N | VAL | B | 249 | 12.722 | 34.380 | -8.478 | 1.00 | 24.22 |
| 7973 | CA | VAL | B | 249 | 12.133 | 35.431 | -9.334 | 1.00 | 25.09 |
| 7975 | CB | BVAL | B | 249 | 13.207 | 36.455 | -9.871 | 0.35 | 24.92 |
| 7976 | CB | AVAL | B | 249 | 13.180 | 36.479 | -9.849 | 0.65 | 25.18 |
| 7979 | CG1 | BVAL | B | 249 | 14.454 | 35.767 | -10.368 | 0.35 | 24.74 |
| 7980 | CG1 | AVAL | B | 249 | 14.270 | 36.727 | -8.817 | 0.65 | 24.27 |
| 7987 | CG2 | BVAL | B | 249 | 12.633 | 37.361 | -10.975 | 0.35 | 23.96 |
| 7988 | CG2 | AVAL | B | 249 | 13.775 | 36.088 | -11.166 | 0.65 | 25.87 |
| 7995 | C | VAL | B | 249 | 11.271 | 34.851 | -10.474 | 1.00 | 25.74 |
| 7996 | O | VAL | B | 249 | 10.167 | 35.330 | -10.688 | 1.00 | 25.89 |
| 7997 | N | VAL | B | 250 | 11.745 | 33.812 | -11.160 | 1.00 | 26.96 |
| 7999 | CA | VAL | B | 250 | 11.065 | 33.282 | -12.350 | 1.00 | 27.89 |
| 8001 | CB | VAL | B | 250 | 12.069 | 32.914 | -13.472 | 1.00 | 28.15 |
| 8003 | CG1 | VAL | B | 250 | 12.996 | 34.083 | -13.769 | 1.00 | 29.48 |
| 8007 | CG2 | VAL | B | 250 | 12.852 | 31.642 | -13.143 | 1.00 | 28.31 |
| 8011 | C | VAL | B | 250 | 10.158 | 32.066 | -12.136 | 1.00 | 28.41 |
| 8012 | O | VAL | B | 250 | 9.330 | 31.776 | -12.983 | 1.00 | 28.51 |
| 8013 | N | GLY | B | 251 | 10.331 | 31.335 | -11.038 | 1.00 | 29.07 |
| 8015 | CA | GLY | B | 251 | 9.583 | 30.107 | -10.813 | 1.00 | 29.72 |
| 8018 | C | GLY | B | 251 | 8.131 | 30.378 | -10.460 | 1.00 | 30.36 |
| 8019 | O | GLY | B | 251 | 7.793 | 31.482 | -10.070 | 1.00 | 31.39 |
| 8020 | N | ASP | B | 252 | 7.276 | 29.376 | -10.613 | 1.00 | 30.83 |
| 8022 | CA | ASP | B | 252 | 5.885 | 29.465 | -10.194 | 1.00 | 31.66 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 8024 | CB | ASP | B | 252 | 4.996 | 28.632 | -11.128 | 1.00 | 32.32 |
| 8027 | CG | ASP | B | 252 | 3.527 | 29.006 | -11.027 | 1.00 | 35.80 |
| 8028 | OD1 | ASP | B | 252 | 2.981 | 29.516 | -12.041 | 1.00 | 41.36 |
| 8029 | OD2 | ASP | B | 252 | 2.818 | 28.820 | -9.997 | 1.00 | 39.19 |
| 8030 | C | ASP | B | 252 | 5.782 | 28.894 | -8.790 | 1.00 | 30.65 |
| 8031 | O | ASP | B | 252 | 6.321 | 27.842 | -8.546 | 1.00 | 30.56 |
| 8032 | N | THR | B | 253 | 5.072 | 29.572 | -7.892 | 1.00 | 29.92 |
| 8034 | CA | THR | B | 253 | 4.846 | 29.080 | -6.533 | 1.00 | 29.76 |
| 8036 | CB | THR | B | 253 | 3.814 | 29.975 | -5.811 | 1.00 | 29.87 |
| 8038 | OG1 | THR | B | 253 | 4.378 | 31.272 | -5.593 | 1.00 | 31.54 |
| 8040 | CG2 | THR | B | 253 | 3.502 | 29.459 | -4.399 | 1.00 | 30.40 |
| 8044 | C | THR | B | 253 | 4.401 | 27.611 | -6.492 | 1.00 | 28.88 |
| 8045 | O | THR | B | 253 | 4.911 | 26.844 | -5.685 | 1.00 | 28.30 |
| 8046 | N | ALA | B | 254 | 3.465 | 27.222 | -7.358 | 1.00 | 28.23 |
| 8048 | CA | ALA | B | 254 | 2.932 | 25.852 | -7.367 | 1.00 | 28.33 |
| 8050 | CB | ALA | B | 254 | 1.809 | 25.708 | -8.391 | 1.00 | 28.17 |
| 8054 | C | ALA | B | 254 | 4.007 | 24.805 | -7.644 | 1.00 | 28.26 |
| 8055 | O | ALA | B | 254 | 3.925 | 23.687 | -7.143 | 1.00 | 28.69 |
| 8056 | N | THR | B | 255 | 4.985 | 25.172 | -8.466 | 1.00 | 27.77 |
| 8058 | CA | THR | B | 255 | 6.091 | 24.292 | -8.824 | 1.00 | 27.75 |
| 8060 | CB | THR | B | 255 | 6.638 | 24.726 | -10.188 | 1.00 | 27.90 |
| 8062 | OG1 | THR | B | 255 | 5.596 | 24.624 | -11.164 | 1.00 | 30.21 |
| 8064 | CG2 | THR | B | 255 | 7.706 | 23.767 | -10.678 | 1.00 | 28.58 |
| 8068 | C | THR | B | 255 | 7.223 | 24.275 | -7.773 | 1.00 | 26.85 |
| 8069 | O | THR | B | 255 | 7.671 | 23.202 | -7.356 | 1.00 | 26.31 |
| 8070 | N | LEU | B | 256 | 7.654 | 25.463 | -7.348 | 1.00 | 25.98 |
| 8072 | CA | LEU | B | 256 | 8.706 | 25.627 | -6.328 | 1.00 | 25.67 |
| 8074 | CB | LEU | B | 256 | 8.994 | 27.116 | -6.091 | 1.00 | 25.92 |
| 8077 | CG | LEU | B | 256 | 9.408 | 28.030 | -7.239 | 1.00 | 27.52 |
| 8079 | CD1 | LEU | B | 256 | 9.656 | 29.433 | -6.691 | 1.00 | 27.93 |
| 8083 | CD2 | LEU | B | 256 | 10.625 | 27.516 | -7.954 | 1.00 | 28.70 |
| 8087 | C | LEU | B | 256 | 8.359 | 25.039 | -4.965 | 1.00 | 24.61 |
| 8088 | O | LEU | B | 256 | 9.244 | 24.625 | -4.217 | 1.00 | 22.99 |
| 8089 | N | GLY | B | 257 | 7.077 | 25.078 | -4.612 | 1.00 | 23.96 |
| 8091 | CA | GLY | B | 257 | 6.636 | 24.759 | -3.265 | 1.00 | 23.66 |
| 8094 | C | GLY | B | 257 | 6.808 | 25.892 | -2.263 | 1.00 | 23.66 |
| 8095 | O | GLY | B | 257 | 6.449 | 25.748 | -1.105 | 1.00 | 23.25 |
| 8096 | N | LYS | B | 258 | 7.310 | 27.036 | -2.721 | 1.00 | 23.45 |
| 8098 | CA | LYS | B | 258 | 7.499 | 28.207 | -1.881 | 1.00 | 23.55 |
| 8100 | CB | LYS | B | 258 | 8.913 | 28.217 | -1.262 | 1.00 | 23.19 |
| 8103 | CG | LYS | B | 258 | 10.065 | 28.100 | -2.279 | 1.00 | 22.81 |
| 8106 | CD | LYS | B | 258 | 11.443 | 27.892 | -1.587 | 1.00 | 21.30 |
| 8109 | CE | LYS | B | 258 | 12.575 | 28.125 | -2.537 | 1.00 | 19.95 |
| 8112 | NZ | LYS | B | 258 | 13.876 | 27.549 | -2.087 | 1.00 | 18.06 |
| 8116 | C | LYS | B | 258 | 7.248 | 29.466 | -2.729 | 1.00 | 24.42 |
| 8117 | O | LYS | B | 258 | 7.280 | 29.414 | -3.961 | 1.00 | 24.38 |
| 8118 | N | ARG | B | 259 | 7.024 | 30.592 | -2.066 | 1.00 | 25.44 |
| 8120 | CA | ARG | B | 259 | 6.534 | 31.795 | -2.744 | 1.00 | 26.73 |
| 8122 | CB | ARG | B | 259 | 6.006 | 32.830 | -1.737 | 1.00 | 27.67 |
| 8125 | CG | ARG | B | 259 | 4.510 | 33.101 | -1.907 | 1.00 | 31.24 |
| 8128 | CD | ARG | B | 259 | 3.825 | 33.710 | -0.700 | 1.00 | 35.52 |
| 8131 | NE | ARG | B | 259 | 3.150 | 32.704 | 0.116 | 1.00 | 37.39 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 8133 | CZ | ARG | B | 259 | 2.036 | 32.056 | -0.235 | 1.00 | 39.88 |
| 8134 | NH1 | ARG | B | 259 | 1.451 | 32.263 | -1.417 | 1.00 | 41.43 |
| 8137 | NH2 | ARG | B | 259 | 1.518 | 31.167 | 0.605 | 1.00 | 41.57 |
| 8140 | C | ARG | B | 259 | 7.550 | 32.432 | -3.685 | 1.00 | 25.93 |
| 8141 | O | ARG | B | 259 | 8.642 | 32.852 | -3.283 | 1.00 | 25.79 |
| 8142 | N | GLN | B | 260 | 7.176 | 32.480 | -4.955 | 1.00 | 25.68 |
| 8144 | CA | GLN | B | 260 | 7.848 | 33.323 | -5.931 | 1.00 | 25.41 |
| 8146 | CB | GLN | B | 260 | 7.076 | 33.337 | -7.255 | 1.00 | 25.85 |
| 8149 | CG | BGLN | B | 260 | 7.707 | 34.187 | -8.363 | 0.35 | 25.46 |
| 8150 | CG | AGLN | B | 260 | 7.696 | 34.266 | -8.323 | 0.65 | 26.52 |
| 8155 | CD | BGLN | B | 260 | 7.388 | 35.665 | -8.261 | 0.35 | 25.75 |
| 8156 | CD | AGLN | B | 260 | 6.858 | 34.376 | -9.595 | 0.65 | 29.40 |
| 8157 | OE1 | BGLN | B | 260 | 8.227 | 36.501 | -8.593 | 0.35 | 26.04 |
| 8158 | OE1 | AGLN | B | 260 | 7.335 | 34.901 | -10.609 | 0.65 | 30.77 |
| 8159 | NE2 | BGLN | B | 260 | 6.180 | 35.993 | -7.809 | 0.35 | 25.98 |
| 8160 | NE2 | AGLN | B | 260 | 5.622 | 33.888 | -9.547 | 0.65 | 29.10 |
| 8165 | C | GLN | B | 260 | 7.900 | 34.730 | -5.369 | 1.00 | 24.67 |
| 8166 | O | GLN | B | 260 | 6.942 | 35.184 | -4.755 | 1.00 | 24.03 |
| 8167 | N | GLY | B | 261 | 9.023 | 35.413 | -5.565 | 1.00 | 24.23 |
| 8169 | CA | GLY | B | 261 | 9.107 | 36.829 | -5.264 | 1.00 | 24.15 |
| 8172 | C | GLY | B | 261 | 9.417 | 37.151 | -3.816 | 1.00 | 24.34 |
| 8173 | O | GLY | B | 261 | 9.464 | 38.307 | -3.465 | 1.00 | 24.07 |
| 8174 | N | ALA | B | 262 | 9.656 | 36.142 | -2.983 | 1.00 | 24.66 |
| 8176 | CA | ALA | B | 262 | 9.909 | 36.359 | -1.559 | 1.00 | 25.08 |
| 8178 | CB | ALA | B | 262 | 9.978 | 35.024 | -0.833 | 1.00 | 24.93 |
| 8182 | C | ALA | B | 262 | 11.179 | 37.180 | -1.288 | 1.00 | 25.56 |
| 8183 | O | ALA | B | 262 | 11.213 | 37.979 | -0.353 | 1.00 | 26.42 |
| 8184 | N | ASP | B | 263 | 12.210 | 37.000 | -2.105 | 1.00 | 25.88 |
| 8186 | CA | ASP | B | 263 | 13.466 | 37.739 | -1.932 | 1.00 | 26.25 |
| 8188 | CB | ASP | B | 263 | 14.564 | 37.191 | -2.848 | 1.00 | 26.11 |
| 8191 | CG | ASP | B | 263 | 15.025 | 35.791 | -2.463 | 1.00 | 26.45 |
| 8192 | OD1 | ASP | B | 263 | 14.815 | 35.353 | -1.299 | 1.00 | 26.12 |
| 8193 | OD2 | ASP | B | 263 | 15.602 | 35.054 | -3.292 | 1.00 | 25.40 |
| 8194 | C | ASP | B | 263 | 13.286 | 39.221 | -2.241 | 1.00 | 27.05 |
| 8195 | O | ASP | B | 263 | 13.823 | 40.074 | -1.549 | 1.00 | 26.45 |
| 8196 | N | GLN | B | 264 | 12.545 | 39.520 | -3.304 | 1.00 | 28.65 |
| 8198 | CA | GLN | B | 264 | 12.278 | 40.908 | -3.691 | 1.00 | 29.67 |
| 8200 | CB | BGLN | B | 264 | 11.590 | 40.972 | -5.061 | 0.35 | 29.64 |
| 8201 | CB | AGLN | B | 264 | 11.557 | 40.939 | -5.046 | 0.65 | 30.10 |
| 8206 | CG | BGLN | B | 264 | 12.546 | 40.710 | -6.226 | 0.35 | 29.64 |
| 8207 | CG | AGLN | B | 264 | 11.357 | 42.333 | -5.625 | 0.65 | 31.67 |
| 8212 | CD | BGLN | B | 264 | 11.961 | 41.060 | -7.589 | 0.35 | 29.88 |
| 8213 | CD | AGLN | B | 264 | 9.896 | 42.666 | -5.883 | 0.65 | 33.37 |
| 8214 | OE1 | BGLN | B | 264 | 12.242 | 40.380 | -8.581 | 0.35 | 29.18 |
| 8215 | OE1 | AGLN | B | 264 | 9.502 | 42.893 | -7.025 | 0.65 | 34.64 |
| 8216 | NE2 | BGLN | B | 264 | 11.163 | 42.126 | -7.646 | 0.35 | 29.79 |
| 8217 | NE2 | AGLN | B | 264 | 9.094 | 42.705 | -4.820 | 0.65 | 34.91 |
| 8222 | C | GLN | B | 264 | 11.455 | 41.638 | -2.614 | 1.00 | 29.97 |
| 8223 | O | GLN | B | 264 | 11.755 | 42.780 | -2.274 | 1.00 | 29.34 |
| 8224 | N | GLN | B | 265 | 10.439 | 40.957 | -2.080 | 1.00 | 30.70 |
| 8226 | CA | GLN | B | 265 | 9.658 | 41.427 | -0.922 | 1.00 | 31.61 |
| 8228 | CB | GLN | B | 265 | 8.769 | 40.285 | -0.410 | 1.00 | 32.41 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 8231 | CG | GLN | B | 265 | 7.466 | 40.703 | 0.244 | 1.00 | 35.31 |
| 8234 | CD | GLN | B | 265 | 6.317 | 40.769 | -0.744 | 1.00 | 39.68 |
| 8235 | OE1 | GLN | B | 265 | 5.925 | 41.861 | -1.174 | 1.00 | 43.25 |
| 8236 | NE2 | GLN | B | 265 | 5.780 | 39.605 | -1.119 | 1.00 | 42.40 |
| 8239 | C | GLN | B | 265 | 10.546 | 41.934 | 0.242 | 1.00 | 31.29 |
| 8240 | O | GLN | B | 265 | 10.321 | 43.032 | 0.776 | 1.00 | 31.47 |
| 8241 | N | LEU | B | 266 | 11.552 | 41.135 | 0.612 | 1.00 | 30.18 |
| 8243 | CA | LEU | B | 266 | 12.421 | 41.420 | 1.761 | 1.00 | 29.88 |
| 8245 | CB | LEU | B | 266 | 12.851 | 40.109 | 2.446 | 1.00 | 29.79 |
| 8248 | CG | LEU | B | 266 | 11.792 | 39.268 | 3.160 | 1.00 | 30.18 |
| 8250 | CD1 | LEU | B | 266 | 12.453 | 38.363 | 4.192 | 1.00 | 29.62 |
| 8254 | CD2 | LEU | B | 266 | 10.742 | 40.140 | 3.817 | 1.00 | 31.47 |
| 8258 | C | LEU | B | 266 | 13.681 | 42.207 | 1.413 | 1.00 | 28.94 |
| 8259 | O | LEU | B | 266 | 14.431 | 42.593 | 2.307 | 1.00 | 29.69 |
| 8260 | N | GLY | B | 267 | 13.921 | 42.429 | 0.128 | 1.00 | 27.95 |
| 8262 | CA | GLY | B | 267 | 15.133 | 43.084 | -0.333 | 1.00 | 26.93 |
| 8265 | C | GLY | B | 267 | 16.398 | 42.279 | -0.094 | 1.00 | 25.88 |
| 8266 | O | GLY | B | 267 | 17.436 | 42.845 | 0.261 | 1.00 | 25.61 |
| 8267 | N | LYS | B | 268 | 16.325 | 40.959 | -0.277 | 1.00 | 24.82 |
| 8269 | CA | LYS | B | 268 | 17.501 | 40.115 | -0.136 | 1.00 | 23.75 |
| 8271 | CB | LYS | B | 268 | 17.153 | 38.627 | -0.295 | 1.00 | 23.56 |
| 8274 | CG | LYS | B | 268 | 16.230 | 38.069 | 0.762 | 1.00 | 23.25 |
| 8277 | CD | LYS | B | 268 | 16.916 | 37.862 | 2.096 | 1.00 | 21.56 |
| 8280 | CE | LYS | B | 268 | 15.901 | 37.433 | 3.158 | 1.00 | 23.14 |
| 8283 | NZ | LYS | B | 268 | 16.536 | 37.070 | 4.482 | 1.00 | 21.85 |
| 8287 | C | LYS | B | 268 | 18.515 | 40.497 | -1.195 | 1.00 | 23.58 |
| 8288 | O | LYS | B | 268 | 18.145 | 40.845 | -2.337 | 1.00 | 23.29 |
| 8289 | N | SER | B | 269 | 19.785 | 40.474 | -0.803 | 1.00 | 22.82 |
| 8291 | CA | SER | B | 269 | 20.885 | 40.514 | -1.746 | 1.00 | 22.51 |
| 8293 | CB | SER | B | 269 | 22.206 | 40.785 | -1.035 | 1.00 | 22.93 |
| 8296 | OG | SER | B | 269 | 22.263 | 42.141 | -0.613 | 1.00 | 23.10 |
| 8298 | C | SER | B | 269 | 20.934 | 39.170 | -2.452 | 1.00 | 22.79 |
| 8299 | O | SER | B | 269 | 21.051 | 38.122 | -1.784 | 1.00 | 22.61 |
| 8300 | N | THR | B | 270 | 20.786 | 39.194 | -3.782 | 1.00 | 21.90 |
| 8302 | CA | THR | B | 270 | 20.764 | 37.973 | -4.593 | 1.00 | 22.01 |
| 8304 | CB | THR | B | 270 | 19.304 | 37.496 | -4.909 | 1.00 | 22.17 |
| 8306 | OG1 | THR | B | 270 | 18.667 | 38.392 | -5.827 | 1.00 | 23.42 |
| 8308 | CG2 | THR | B | 270 | 18.386 | 37.525 | -3.707 | 1.00 | 21.68 |
| 8312 | C | THR | B | 270 | 21.499 | 38.175 | -5.908 | 1.00 | 21.99 |
| 8313 | O | THR | B | 270 | 21.731 | 39.306 | -6.354 | 1.00 | 21.16 |
| 8314 | N | TYR | B | 271 | 21.841 | 37.066 | -6.553 | 1.00 | 21.84 |
| 8316 | CA | TYR | B | 271 | 22.470 | 37.134 | -7.864 | 1.00 | 22.04 |
| 8318 | CB | TYR | B | 271 | 22.959 | 35.754 | -8.319 | 1.00 | 21.34 |
| 8321 | CG | TYR | B | 271 | 24.340 | 35.435 | -7.803 | 1.00 | 20.33 |
| 8322 | CD1 | TYR | B | 271 | 25.430 | 35.422 | -8.654 | 1.00 | 20.38 |
| 8324 | CE1 | TYR | B | 271 | 26.686 | 35.129 | -8.197 | 1.00 | 20.95 |
| 8326 | CZ | TYR | B | 271 | 26.877 | 34.859 | -6.866 | 1.00 | 20.10 |
| 8327 | OH | TYR | B | 271 | 28.142 | 34.576 | -6.417 | 1.00 | 24.40 |
| 8329 | CE2 | TYR | B | 271 | 25.818 | 34.876 | -5.989 | 1.00 | 19.89 |
| 8331 | CD2 | TYR | B | 271 | 24.561 | 35.161 | -6.455 | 1.00 | 18.52 |
| 8333 | C | TYR | B | 271 | 21.588 | 37.816 | -8.933 | 1.00 | 22.40 |
| 8334 | O | TYR | B | 271 | 22.075 | 38.711 | -9.612 | 1.00 | 22.20 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 8335 | N | PRO | B | 272 | 20.328 | 37.413 | -9.102 | 1.00 | 22.68 |
| 8336 | CA | PRO | B | 272 | 19.448 | 38.083 | -10.073 | 1.00 | 23.28 |
| 8338 | CB | PRO | B | 272 | 18.131 | 37.309 | -9.984 | 1.00 | 23.44 |
| 8341 | CG | PRO | B | 272 | 18.438 | 36.064 | -9.253 | 1.00 | 23.26 |
| 8344 | CD | PRO | B | 272 | 19.635 | 36.319 | -8.412 | 1.00 | 23.08 |
| 8347 | C | PRO | B | 272 | 19.193 | 39.550 | -9.744 | 1.00 | 23.45 |
| 8348 | O | PRO | B | 272 | 19.084 | 40.350 | -10.668 | 1.00 | 23.18 |
| 8349 | N | ALA | B | 273 | 19.099 | 39.890 | -8.460 | 1.00 | 23.47 |
| 8351 | CA | ALA | B | 273 | 18.821 | 41.268 | -8.062 | 1.00 | 23.58 |
| 8353 | CB | ALA | B | 273 | 18.569 | 41.386 | -6.560 | 1.00 | 23.84 |
| 8357 | C | ALA | B | 273 | 19.962 | 42.155 | -8.483 | 1.00 | 23.82 |
| 8358 | O | ALA | B | 273 | 19.742 | 43.216 | -9.062 | 1.00 | 24.38 |
| 8359 | N | LEU | B | 274 | 21.184 | 41.692 | -8.247 | 1.00 | 23.53 |
| 8361 | CA | LEU | B | 274 | 22.375 | 42.447 | -8.586 | 1.00 | 23.59 |
| 8363 | CB | LEU | B | 274 | 23.566 | 41.908 | -7.798 | 1.00 | 23.51 |
| 8366 | CG | LEU | B | 274 | 24.934 | 42.511 | -8.113 | 1.00 | 23.92 |
| 8368 | CD1 | LEU | B | 274 | 24.947 | 44.021 | -7.830 | 1.00 | 24.92 |
| 8372 | CD2 | LEU | B | 274 | 26.012 | 41.800 | -7.318 | 1.00 | 24.12 |
| 8376 | C | LEU | B | 274 | 22.704 | 42.437 | -10.082 | 1.00 | 23.25 |
| 8377 | O | LEU | B | 274 | 22.964 | 43.479 | -10.664 | 1.00 | 23.31 |
| 8378 | N | LEU | B | 275 | 22.693 | 41.253 | -10.683 | 1.00 | 22.76 |
| 8380 | CA | LEU | B | 275 | 23.281 | 41.018 | -11.995 | 1.00 | 22.56 |
| 8382 | CB | LEU | B | 275 | 24.093 | 39.726 | -11.983 | 1.00 | 22.53 |
| 8385 | CG | LEU | B | 275 | 25.314 | 39.686 | -11.062 | 1.00 | 24.16 |
| 8387 | CD1 | LEU | B | 275 | 25.881 | 38.277 | -11.022 | 1.00 | 25.08 |
| 8391 | CD2 | LEU | B | 275 | 26.394 | 40.674 | -11.518 | 1.00 | 25.88 |
| 8395 | C | LEU | B | 275 | 22.237 | 40.925 | -13.089 | 1.00 | 21.93 |
| 8396 | O | LEU | B | 275 | 22.567 | 40.925 | -14.273 | 1.00 | 21.98 |
| 8397 | N | GLY | B | 276 | 20.981 | 40.880 | -12.696 | 1.00 | 21.10 |
| 8399 | CA | GLY | B | 276 | 19.925 | 40.537 | -13.619 | 1.00 | 21.48 |
| 8402 | C | GLY | B | 276 | 19.923 | 39.035 | -13.860 | 1.00 | 21.79 |
| 8403 | O | GLY | B | 276 | 20.883 | 38.320 | -13.530 | 1.00 | 20.41 |
| 8404 | N | LEU | B | 277 | 18.831 | 38.570 | -14.445 | 1.00 | 22.27 |
| 8406 | CA | LEU | B | 277 | 18.587 | 37.145 | -14.645 | 1.00 | 23.11 |
| 8408 | CB | LEU | B | 277 | 17.169 | 36.923 | -15.161 | 1.00 | 23.57 |
| 8411 | CG | LEU | B | 277 | 16.145 | 36.966 | -14.051 | 1.00 | 23.96 |
| 8413 | CD1 | LEU | B | 277 | 14.712 | 36.988 | -14.638 | 1.00 | 25.68 |
| 8417 | CD2 | LEU | B | 277 | 16.375 | 35.748 | -13.152 | 1.00 | 24.82 |
| 8421 | C | LEU | B | 277 | 19.554 | 36.493 | -15.601 | 1.00 | 23.62 |
| 8422 | O | LEU | B | 277 | 19.999 | 35.393 | -15.348 | 1.00 | 22.96 |
| 8423 | N | GLU | B | 278 | 19.885 | 37.158 | -16.704 | 1.00 | 24.28 |
| 8425 | CA | GLU | B | 278 | 20.703 | 36.498 | -17.715 | 1.00 | 25.35 |
| 8427 | CB | GLU | B | 278 | 20.712 | 37.237 | -19.049 | 1.00 | 26.22 |
| 8430 | CG | GLU | B | 278 | 21.247 | 36.373 | -20.184 | 1.00 | 30.72 |
| 8433 | CD | GLU | B | 278 | 20.177 | 35.523 | -20.858 | 1.00 | 36.13 |
| 8434 | OE1 | GLU | B | 278 | 19.801 | 35.857 | -22.020 | 1.00 | 40.61 |
| 8435 | OE2 | GLU | B | 278 | 19.725 | 34.513 | -20.244 | 1.00 | 38.13 |
| 8436 | C | GLU | B | 278 | 22.116 | 36.293 | -17.220 | 1.00 | 24.46 |
| 8437 | O | GLU | B | 278 | 22.658 | 35.215 | -17.405 | 1.00 | 23.99 |
| 8438 | N | GLN | B | 279 | 22.707 | 37.305 | -16.582 | 1.00 | 23.54 |
| 8440 | CA | GLN | B | 279 | 24.052 | 37.148 | -16.019 | 1.00 | 23.89 |
| 8442 | CB | GLN | B | 279 | 24.640 | 38.488 | -15.569 | 1.00 | 23.95 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 8445 | CG | GLN | B | 279 | 25.057 | 39.407 | -16.701 | 1.00 | 26.62 |
| 8448 | CD | GLN | B | 279 | 25.436 | 40.804 | -16.197 | 1.00 | 29.62 |
| 8449 | OE1 | GLN | B | 279 | 26.041 | 40.939 | -15.140 | 1.00 | 29.56 |
| 8450 | NE2 | GLN | B | 279 | 25.046 | 41.834 | -16.941 | 1.00 | 32.63 |
| 8453 | C | GLN | B | 279 | 24.042 | 36.157 | -14.848 | 1.00 | 23.16 |
| 8454 | O | GLN | B | 279 | 24.994 | 35.428 | -14.656 | 1.00 | 23.94 |
| 8455 | N | ALA | B | 280 | 22.968 | 36.130 | -14.071 | 1.00 | 22.86 |
| 8457 | CA | ALA | B | 280 | 22.852 | 35.161 | -12.985 | 1.00 | 22.78 |
| 8459 | CB | ALA | B | 280 | 21.591 | 35.413 | -12.169 | 1.00 | 22.56 |
| 8463 | C | ALA | B | 280 | 22.848 | 33.738 | -13.565 | 1.00 | 22.60 |
| 8464 | O | ALA | B | 280 | 23.542 | 32.873 | -13.071 | 1.00 | 22.64 |
| 8465 | N | ARG | B | 281 | 22.085 | 33.520 | -14.632 | 1.00 | 22.89 |
| 8467 | CA | ARG | B | 281 | 22.048 | 32.213 | -15.299 | 1.00 | 23.30 |
| 8469 | CB | ARG | B | 281 | 21.012 | 32.205 | -16.431 | 1.00 | 23.67 |
| 8472 | CG | ARG | B | 281 | 19.594 | 32.090 | -15.944 | 1.00 | 25.28 |
| 8475 | CD | ARG | B | 281 | 18.542 | 32.199 | -17.031 | 1.00 | 27.92 |
| 8478 | NE | ARG | B | 281 | 17.209 | 31.888 | -16.503 | 1.00 | 30.36 |
| 8480 | CZ | ARG | B | 281 | 16.104 | 32.616 | -16.697 | 1.00 | 32.35 |
| 8481 | NH1 | ARG | B | 281 | 16.121 | 33.727 | -17.423 | 1.00 | 31.95 |
| 8484 | NH2 | ARG | B | 281 | 14.954 | 32.217 | -16.160 | 1.00 | 34.03 |
| 8487 | C | ARG | B | 281 | 23.424 | 31.827 | -15.854 | 1.00 | 23.20 |
| 8488 | O | ARG | B | 281 | 23.843 | 30.669 | -15.783 | 1.00 | 22.27 |
| 8489 | N | LYS | B | 282 | 24.111 | 32.807 | -16.421 | 1.00 | 23.01 |
| 8491 | CA | LYS | B | 282 | 25.418 | 32.595 | -16.998 | 1.00 | 22.90 |
| 8493 | CB | LYS | B | 282 | 25.870 | 33.833 | -17.774 | 1.00 | 23.16 |
| 8496 | CG | LYS | B | 282 | 27.307 | 33.794 | -18.251 | 1.00 | 24.89 |
| 8499 | CD | LYS | B | 282 | 27.542 | 32.619 | -19.190 | 1.00 | 28.29 |
| 8502 | CE | LYS | B | 282 | 28.672 | 32.892 | -20.166 | 1.00 | 29.58 |
| 8505 | NZ | LYS | B | 282 | 29.948 | 33.113 | -19.451 | 1.00 | 30.99 |
| 8509 | C | LYS | B | 282 | 26.422 | 32.253 | -15.893 | 1.00 | 22.40 |
| 8510 | O | LYS | B | 282 | 27.270 | 31.400 | -16.086 | 1.00 | 22.05 |
| 8511 | N | LYS | B | 283 | 26.312 | 32.901 | -14.742 | 1.00 | 21.92 |
| 8513 | CA | LYS | B | 283 | 27.191 | 32.604 | -13.612 | 1.00 | 22.26 |
| 8515 | CB | LYS | B | 283 | 26.959 | 33.566 | -12.444 | 1.00 | 22.86 |
| 8518 | CG | LYS | B | 283 | 27.325 | 35.029 | -12.759 | 1.00 | 26.57 |
| 8521 | CD | LYS | B | 283 | 28.574 | 35.530 | -12.019 | 1.00 | 30.08 |
| 8524 | CE | LYS | B | 283 | 29.067 | 36.885 | -12.583 | 1.00 | 31.95 |
| 8527 | NZ | LYS | B | 283 | 30.540 | 37.060 | -12.449 | 1.00 | 33.10 |
| 8531 | C | LYS | B | 283 | 26.982 | 31.151 | -13.175 | 1.00 | 21.47 |
| 8532 | O | LYS | B | 283 | 27.939 | 30.422 | -12.944 | 1.00 | 21.43 |
| 8533 | N | ALA | B | 284 | 25.725 | 30.729 | -13.101 | 1.00 | 20.57 |
| 8535 | CA | ALA | B | 284 | 25.408 | 29.366 | -12.697 | 1.00 | 20.64 |
| 8537 | CB | ALA | B | 284 | 23.881 | 29.171 | -12.552 | 1.00 | 20.42 |
| 8541 | C | ALA | B | 284 | 25.990 | 28.377 | -13.699 | 1.00 | 20.27 |
| 8542 | O | ALA | B | 284 | 26.607 | 27.383 | -13.306 | 1.00 | 19.24 |
| 8543 | N | ARG | B | 285 | 25.819 | 28.639 | -14.990 | 1.00 | 20.74 |
| 8545 | CA | ARG | B | 285 | 26.307 | 27.695 | -15.997 | 1.00 | 21.12 |
| 8547 | CB | ARG | B | 285 | 25.765 | 28.003 | -17.392 | 1.00 | 21.76 |
| 8550 | CG | ARG | B | 285 | 26.088 | 26.897 | -18.402 | 1.00 | 22.89 |
| 8553 | CD | ARG | B | 285 | 25.654 | 27.222 | -19.814 | 1.00 | 25.89 |
| 8556 | NE | ARG | B | 285 | 26.498 | 28.272 | -20.382 | 1.00 | 26.63 |
| 8558 | CZ | ARG | B | 285 | 26.296 | 28.833 | -21.562 | 1.00 | 26.13 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 8559 | NH1 | ARG | B | 285 | 25.253 | 28.490 | -22.311 | 1.00 | 24.20 |
| 8562 | NH2 | ARG | B | 285 | 27.138 | 29.760 | -21.981 | 1.00 | 25.45 |
| 8565 | C | ARG | B | 285 | 27.831 | 27.650 | -16.001 | 1.00 | 21.30 |
| 8566 | O | ARG | B | 285 | 28.416 | 26.590 | -16.177 | 1.00 | 21.07 |
| 8567 | N | ASP | B | 286 | 28.461 | 28.795 | -15.766 | 1.00 | 21.40 |
| 8569 | CA | ASP | B | 286 | 29.915 | 28.874 | -15.595 | 1.00 | 21.87 |
| 8571 | CB | ASP | B | 286 | 30.335 | 30.327 | -15.313 | 1.00 | 22.54 |
| 8574 | CG | ASP | B | 286 | 30.370 | 31.200 | -16.579 | 1.00 | 25.24 |
| 8575 | OD1 | ASP | B | 286 | 30.630 | 32.424 | -16.457 | 1.00 | 28.05 |
| 8576 | OD2 | ASP | B | 286 | 30.138 | 30.759 | -17.724 | 1.00 | 26.91 |
| 8577 | C | ASP | B | 286 | 30.401 | 27.958 | -14.456 | 1.00 | 21.04 |
| 8578 | O | ASP | B | 286 | 31.440 | 27.297 | -14.562 | 1.00 | 20.76 |
| 8579 | N | LEU | B | 287 | 29.633 | 27.922 | -13.372 | 1.00 | 20.21 |
| 8581 | CA | LEU | B | 287 | 29.994 | 27.151 | -12.188 | 1.00 | 19.69 |
| 8583 | CB | LEU | B | 287 | 29.141 | 27.569 | -10.992 | 1.00 | 19.82 |
| 8586 | CG | LEU | B | 287 | 29.530 | 28.953 | -10.452 | 1.00 | 18.53 |
| 8588 | CD1 | LEU | B | 287 | 28.423 | 29.532 | -9.589 | 1.00 | 19.63 |
| 8592 | CD2 | LEU | B | 287 | 30.812 | 28.869 | -9.646 | 1.00 | 19.99 |
| 8596 | C | LEU | B | 287 | 29.838 | 25.670 | -12.468 | 1.00 | 19.73 |
| 8597 | O | LEU | B | 287 | 30.671 | 24.889 | -12.094 | 1.00 | 20.05 |
| 8598 | N | ILE | B | 288 | 28.774 | 25.295 | -13.150 | 1.00 | 20.33 |
| 8600 | CA | ILE | B | 288 | 28.597 | 23.906 | -13.555 | 1.00 | 21.14 |
| 8602 | CB | ILE | B | 288 | 27.190 | 23.672 | -14.076 | 1.00 | 21.02 |
| 8604 | CG1 | ILE | B | 288 | 26.178 | 23.925 | -12.949 | 1.00 | 22.56 |
| 8607 | CD1 | ILE | B | 288 | 26.532 | 23.265 | -11.610 | 1.00 | 22.71 |
| 8611 | CG2 | ILE | B | 288 | 27.041 | 22.244 | -14.624 | 1.00 | 21.66 |
| 8615 | C | ILE | B | 288 | 29.659 | 23.477 | -14.566 | 1.00 | 21.32 |
| 8616 | O | ILE | B | 288 | 30.149 | 22.359 | -14.488 | 1.00 | 21.92 |
| 8617 | N | ASP | B | 289 | 30.032 | 24.358 | -15.487 | 1.00 | 21.87 |
| 8619 | CA | ASP | B | 289 | 31.112 | 24.056 | -16.430 | 1.00 | 22.32 |
| 8621 | CB | ASP | B | 289 | 31.436 | 25.261 | -17.330 | 1.00 | 22.60 |
| 8624 | CG | ASP | B | 289 | 30.410 | 25.503 | -18.417 | 1.00 | 23.70 |
| 8625 | OD1 | ASP | B | 289 | 30.445 | 26.623 | -18.989 | 1.00 | 26.27 |
| 8626 | OD2 | ASP | B | 289 | 29.548 | 24.676 | -18.786 | 1.00 | 22.23 |
| 8627 | C | ASP | B | 289 | 32.369 | 23.705 | -15.624 | 1.00 | 22.25 |
| 8628 | O | ASP | B | 289 | 33.066 | 22.756 | -15.928 | 1.00 | 21.47 |
| 8629 | N | ASP | B | 290 | 32.636 | 24.490 | -14.588 | 1.00 | 22.34 |
| 8631 | CA | ASP | B | 290 | 33.793 | 24.291 | -13.731 | 1.00 | 23.23 |
| 8633 | CB | ASP | B | 290 | 33.980 | 25.509 | -12.820 | 1.00 | 23.34 |
| 8636 | CG | ASP | B | 290 | 35.161 | 25.368 | -11.918 | 1.00 | 26.31 |
| 8637 | OD1 | ASP | B | 290 | 36.305 | 25.530 | -12.420 | 1.00 | 28.34 |
| 8638 | OD2 | ASP | B | 290 | 35.037 | 25.088 | -10.697 | 1.00 | 28.06 |
| 8639 | C | ASP | B | 290 | 33.670 | 22.986 | -12.925 | 1.00 | 22.69 |
| 8640 | O | ASP | B | 290 | 34.641 | 22.234 | -12.816 | 1.00 | 22.49 |
| 8641 | N | ALA | B | 291 | 32.474 | 22.703 | -12.405 | 1.00 | 22.19 |
| 8643 | CA | ALA | B | 291 | 32.204 | 21.431 | -11.725 | 1.00 | 22.57 |
| 8645 | CB | ALA | B | 291 | 30.752 | 21.361 | -11.263 | 1.00 | 22.03 |
| 8649 | C | ALA | B | 291 | 32.524 | 20.233 | -12.631 | 1.00 | 22.99 |
| 8650 | O | ALA | B | 291 | 33.151 | 19.270 | -12.190 | 1.00 | 22.66 |
| 8651 | N | ARG | B | 292 | 32.115 | 20.321 | -13.895 | 1.00 | 23.78 |
| 8653 | CA | ARG | B | 292 | 32.394 | 19.283 | -14.883 | 1.00 | 25.16 |
| 8655 | CB | ARG | B | 292 | 31.628 | 19.550 | -16.180 | 1.00 | 25.91 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 8658 | CG | ARG | B | 292 | 30.138 | 19.170 | -16.097 | 1.00 | 28.32 |
| 8661 | CD | BARG | B | 292 | 29.468 | 18.992 | -17.466 | 0.35 | 29.52 |
| 8662 | CD | AARG | B | 292 | 29.453 | 19.007 | -17.451 | 0.65 | 30.92 |
| 8667 | NE | BARG | B | 292 | 29.262 | 20.264 | -18.163 | 0.35 | 29.83 |
| 8668 | NE | AARG | B | 292 | 28.271 | 18.146 | -17.365 | 0.65 | 31.71 |
| 8671 | CZ | BARG | B | 292 | 28.839 | 20.386 | -19.423 | 0.35 | 30.53 |
| 8672 | CZ | AARG | B | 292 | 28.231 | 16.856 | -17.684 | 0.65 | 33.32 |
| 8673 | NH1 | BARG | B | 292 | 28.567 | 19.313 | -20.165 | 0.35 | 30.23 |
| 8674 | NH1 | AARG | B | 292 | 29.309 | 16.209 | -18.125 | 0.65 | 33.00 |
| 8679 | NH2 | BARG | B | 292 | 28.688 | 21.596 | -19.951 | 0.35 | 30.87 |
| 8680 | NH2 | AARG | B | 292 | 27.089 | 16.195 | -17.563 | 0.65 | 33.96 |
| 8685 | C | ARG | B | 292 | 33.894 | 19.108 | -15.170 | 1.00 | 25.22 |
| 8686 | O | ARG | B | 292 | 34.349 | 17.988 | -15.388 | 1.00 | 24.81 |
| 8687 | N | GLN | B | 293 | 34.651 | 20.204 | -15.171 | 1.00 | 25.23 |
| 8689 | CA | GLN | B | 293 | 36.100 | 20.116 | -15.322 | 1.00 | 25.93 |
| 8691 | CB | GLN | B | 293 | 36.756 | 21.497 | -15.472 | 1.00 | 26.28 |
| 8694 | CG | GLN | B | 293 | 36.425 | 22.206 | -16.775 | 1.00 | 29.31 |
| 8697 | CD | GLN | B | 293 | 37.009 | 21.533 | -18.012 | 1.00 | 32.74 |
| 8698 | OE1 | GLN | B | 293 | 38.047 | 20.880 | -17.945 | 1.00 | 35.76 |
| 8699 | NE2 | GLN | B | 293 | 36.340 | 21.706 | -19.144 | 1.00 | 35.59 |
| 8702 | C | GLN | B | 293 | 36.706 | 19.364 | -14.131 | 1.00 | 25.31 |
| 8703 | O | GLN | B | 293 | 37.565 | 18.521 | -14.333 | 1.00 | 24.00 |
| 8704 | N | SER | B | 294 | 36.241 | 19.658 | -12.905 | 1.00 | 25.12 |
| 8706 | CA | SER | B | 294 | 36.665 | 18.911 | -11.720 | 1.00 | 25.39 |
| 8708 | CB | SER | B | 294 | 36.105 | 19.510 | -10.414 | 1.00 | 25.38 |
| 8711 | OG | SER | B | 294 | 36.557 | 20.834 | -10.215 | 1.00 | 24.82 |
| 8713 | C | SER | B | 294 | 36.289 | 17.433 | -11.820 | 1.00 | 25.78 |
| 8714 | O | SER | B | 294 | 37.077 | 16.569 | -11.459 | 1.00 | 25.49 |
| 8715 | N | LEU | B | 295 | 35.098 | 17.125 | -12.321 | 1.00 | 26.38 |
| 8717 | CA | LEU | B | 295 | 34.709 | 15.726 | -12.441 | 1.00 | 27.10 |
| 8719 | CB | LEU | B | 295 | 33.237 | 15.580 | -12.838 | 1.00 | 26.93 |
| 8722 | CG | LEU | B | 295 | 32.258 | 15.977 | -11.729 | 1.00 | 25.30 |
| 8724 | CD1 | LEU | B | 295 | 30.821 | 15.804 | -12.200 | 1.00 | 25.85 |
| 8728 | CD2 | LEU | B | 295 | 32.524 | 15.189 | -10.431 | 1.00 | 25.23 |
| 8732 | C | LEU | B | 295 | 35.635 | 14.995 | -13.425 | 1.00 | 28.16 |
| 8733 | O | LEU | B | 295 | 35.998 | 13.854 | -13.186 | 1.00 | 28.16 |
| 8734 | N | LYS | B | 296 | 36.053 | 15.677 | -14.487 | 1.00 | 29.02 |
| 8736 | CA | LYS | B | 296 | 36.961 | 15.096 | -15.481 | 1.00 | 30.79 |
| 8738 | CB | LYS | B | 296 | 37.313 | 16.118 | -16.587 | 1.00 | 30.97 |
| 8741 | CG | LYS | B | 296 | 36.966 | 15.687 | -18.011 | 1.00 | 33.97 |
| 8744 | CD | LYS | B | 296 | 36.614 | 16.900 | -18.921 | 1.00 | 36.64 |
| 8747 | CE | LYS | B | 296 | 35.099 | 17.019 | -19.182 | 1.00 | 37.79 |
| 8750 | NZ | LYS | B | 296 | 34.637 | 18.445 | -19.343 | 1.00 | 38.84 |
| 8754 | C | LYS | B | 296 | 38.244 | 14.611 | -14.809 | 1.00 | 31.28 |
| 8755 | O | LYS | B | 296 | 38.750 | 13.544 | -15.141 | 1.00 | 31.44 |
| 8756 | N | GLN | B | 297 | 38.759 | 15.401 | -13.869 | 1.00 | 32.13 |
| 8758 | CA | GLN | B | 297 | 39.978 | 15.054 | -13.152 | 1.00 | 33.58 |
| 8760 | CB | GLN | B | 297 | 40.470 | 16.251 | -12.326 | 1.00 | 33.80 |
| 8763 | CG | GLN | B | 297 | 40.818 | 17.493 | -13.167 | 1.00 | 35.12 |
| 8766 | CD | GLN | B | 297 | 40.846 | 18.775 | -12.353 | 1.00 | 36.83 |
| 8767 | OE1 | GLN | B | 297 | 41.175 | 18.756 | -11.168 | 1.00 | 36.95 |
| 8768 | NE2 | GLN | B | 297 | 40.495 | 19.893 | -12.985 | 1.00 | 38.40 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 8771 | C | GLN | B | 297 | 39.800 | 13.810 | -12.265 | 1.00 | 34.42 |
| 8772 | O | GLN | B | 297 | 40.764 | 13.098 | -12.013 | 1.00 | 34.62 |
| 8773 | N | LEU | B | 298 | 38.577 | 13.568 | -11.784 | 1.00 | 35.42 |
| 8775 | CA | LEU | B | 298 | 38.248 | 12.364 | -10.999 | 1.00 | 36.35 |
| 8777 | CB | LEU | B | 298 | 36.931 | 12.542 | -10.251 | 1.00 | 36.39 |
| 8780 | CG | LEU | B | 298 | 36.924 | 13.515 | -9.082 | 1.00 | 36.49 |
| 8782 | CD1 | LEU | B | 298 | 35.562 | 13.491 | -8.411 | 1.00 | 36.85 |
| 8786 | CD2 | LEU | B | 298 | 38.023 | 13.153 | -8.101 | 1.00 | 36.84 |
| 8790 | C | LEU | B | 298 | 38.141 | 11.088 | -11.820 | 1.00 | 37.54 |
| 8791 | O | LEU | B | 298 | 38.519 | 10.015 | -11.352 | 1.00 | 37.33 |
| 8792 | N | ALA | B | 299 | 37.598 | 11.193 | -13.028 | 1.00 | 38.95 |
| 8794 | CA | ALA | B | 299 | 37.635 | 10.088 | -13.974 | 1.00 | 40.14 |
| 8796 | CB | ALA | B | 299 | 36.587 | 10.291 | -15.078 | 1.00 | 40.36 |
| 8800 | C | ALA | B | 299 | 39.045 | 9.950 | -14.565 | 1.00 | 40.76 |
| 8801 | O | ALA | B | 299 | 39.206 | 9.462 | -15.677 | 1.00 | 41.94 |
| 8802 | N | GLU | B | 300 | 40.045 | 10.442 | -13.834 | 1.00 | 41.22 |
| 8804 | CA | GLU | B | 300 | 41.456 | 10.118 | -14.039 | 1.00 | 41.53 |
| 8806 | CB | GLU | B | 300 | 42.240 | 11.402 | -14.318 | 1.00 | 41.94 |
| 8809 | CG | GLU | B | 300 | 43.620 | 11.186 | -14.911 | 1.00 | 44.01 |
| 8812 | CD | GLU | B | 300 | 44.144 | 12.428 | -15.604 | 1.00 | 45.96 |
| 8813 | OE1 | GLU | B | 300 | 44.166 | 13.499 | -14.953 | 1.00 | 48.06 |
| 8814 | OE2 | GLU | B | 300 | 44.528 | 12.332 | -16.794 | 1.00 | 47.73 |
| 8815 | C | GLU | B | 300 | 42.047 | 9.414 | -12.808 | 1.00 | 40.89 |
| 8816 | O | GLU | B | 300 | 43.185 | 8.941 | -12.846 | 1.00 | 41.57 |
| 8817 | N | GLN | B | 301 | 41.295 | 9.399 | -11.705 | 1.00 | 39.90 |
| 8819 | CA | GLN | B | 301 | 41.549 | 8.516 | -10.565 | 1.00 | 38.66 |
| 8821 | CB | GLN | B | 301 | 41.248 | 9.243 | -9.243 | 1.00 | 38.65 |
| 8824 | CG | GLN | B | 301 | 41.958 | 10.592 | -9.083 | 1.00 | 38.47 |
| 8827 | CD | GLN | B | 301 | 41.556 | 11.354 | -7.816 | 1.00 | 37.66 |
| 8828 | OE1 | GLN | B | 301 | 41.179 | 10.751 | -6.807 | 1.00 | 36.11 |
| 8829 | NE2 | GLN | B | 301 | 41.658 | 12.686 | -7.867 | 1.00 | 36.75 |
| 8832 | C | GLN | B | 301 | 40.681 | 7.258 | -10.689 | 1.00 | 37.75 |
| 8833 | O | GLN | B | 301 | 40.432 | 6.560 | -9.698 | 1.00 | 37.50 |
| 8834 | N | SER | B | 302 | 40.220 | 6.995 | -11.914 | 1.00 | 36.44 |
| 8836 | CA | SER | B | 302 | 39.373 | 5.852 | -12.261 | 1.00 | 35.92 |
| 8838 | CB | SER | B | 302 | 40.117 | 4.541 | -12.022 | 1.00 | 36.22 |
| 8841 | OG | SER | B | 302 | 39.666 | 3.572 | -12.955 | 1.00 | 38.05 |
| 8843 | C | SER | B | 302 | 38.003 | 5.810 | -11.566 | 1.00 | 34.56 |
| 8844 | O | SER | B | 302 | 37.551 | 4.753 | -11.143 | 1.00 | 34.47 |
| 8845 | N | LEU | B | 303 | 37.330 | 6.952 | -11.485 | 1.00 | 32.72 |
| 8847 | CA | LEU | B | 303 | 36.060 | 7.022 | -10.773 | 1.00 | 31.10 |
| 8849 | CB | LEU | B | 303 | 36.114 | 8.107 | -9.699 | 1.00 | 30.86 |
| 8852 | CG | LEU | B | 303 | 37.166 | 7.891 | -8.611 | 1.00 | 30.39 |
| 8854 | CD1 | LEU | B | 303 | 37.381 | 9.150 | -7.786 | 1.00 | 30.04 |
| 8858 | CD2 | LEU | B | 303 | 36.771 | 6.739 | -7.721 | 1.00 | 30.69 |
| 8862 | C | LEU | B | 303 | 34.910 | 7.286 | -11.724 | 1.00 | 30.21 |
| 8863 | O | LEU | B | 303 | 35.045 | 8.047 | -12.684 | 1.00 | 29.81 |
| 8864 | N | ASP | B | 304 | 33.776 | 6.655 | -11.425 | 1.00 | 28.91 |
| 8866 | CA | ASP | B | 304 | 32.541 | 6.834 | -12.171 | 1.00 | 28.55 |
| 8868 | CB | ASP | B | 304 | 31.659 | 5.597 | -12.005 | 1.00 | 28.67 |
| 8871 | CG | ASP | B | 304 | 30.377 | 5.661 | -12.823 | 1.00 | 30.58 |
| 8872 | OD1 | ASP | B | 304 | 30.141 | 6.682 | -13.512 | 1.00 | 31.79 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 8873 | OD2 | ASP | B | 304 | 29.534 | 4.729 | -12.815 | 1.00 | 33.35 |
| 8874 | C | ASP | B | 304 | 31.830 | 8.086 | -11.662 | 1.00 | 27.64 |
| 8875 | O | ASP | B | 304 | 31.132 | 8.050 | -10.649 | 1.00 | 26.94 |
| 8876 | N | THR | B | 305 | 32.007 | 9.187 | -12.390 | 1.00 | 26.96 |
| 8878 | CA | THR | B | 305 | 31.424 | 10.478 | -12.020 | 1.00 | 26.33 |
| 8880 | CB | THR | B | 305 | 32.352 | 11.615 | -12.471 | 1.00 | 26.05 |
| 8882 | OG1 | THR | B | 305 | 32.571 | 11.538 | -13.882 | 1.00 | 27.18 |
| 8884 | CG2 | THR | B | 305 | 33.740 | 11.457 | -11.879 | 1.00 | 26.15 |
| 8888 | C | THR | B | 305 | 30.006 | 10.704 | -12.588 | 1.00 | 25.98 |
| 8889 | O | THR | B | 305 | 29.464 | 11.785 | -12.453 | 1.00 | 25.98 |
| 8890 | N | SER | B | 306 | 29.392 | 9.682 | -13.176 | 1.00 | 25.39 |
| 8892 | CA | SER | B | 306 | 28.130 | 9.855 | -13.906 | 1.00 | 25.11 |
| 8894 | CB | SER | B | 306 | 27.672 | 8.535 | -14.531 | 1.00 | 25.29 |
| 8897 | OG | SER | B | 306 | 27.346 | 7.581 | -13.529 | 1.00 | 27.52 |
| 8899 | C | SER | B | 306 | 27.004 | 10.479 | -13.077 | 1.00 | 24.18 |
| 8900 | O | SER | B | 306 | 26.340 | 11.391 | -13.553 | 1.00 | 23.89 |
| 8901 | N | ALA | B | 307 | 26.788 | 10.001 | -11.850 | 1.00 | 23.33 |
| 8903 | CA | ALA | B | 307 | 25.756 | 10.590 | -10.983 | 1.00 | 22.98 |
| 8905 | CB | ALA | B | 307 | 25.555 | 9.776 | -9.736 | 1.00 | 22.98 |
| 8909 | C | ALA | B | 307 | 26.051 | 12.044 | -10.605 | 1.00 | 22.43 |
| 8910 | O | ALA | B | 307 | 25.138 | 12.850 | -10.585 | 1.00 | 21.51 |
| 8911 | N | LEU | B | 308 | 27.321 | 12.361 | -10.309 | 1.00 | 22.10 |
| 8913 | CA | LEU | B | 308 | 27.705 | 13.698 | -9.887 | 1.00 | 21.91 |
| 8915 | CB | LEU | B | 308 | 29.102 | 13.715 | -9.268 | 1.00 | 21.74 |
| 8918 | CG | LEU | B | 308 | 29.295 | 12.964 | -7.951 | 1.00 | 22.89 |
| 8920 | CD1 | LEU | B | 308 | 30.736 | 13.126 | -7.523 | 1.00 | 23.47 |
| 8924 | CD2 | LEU | B | 308 | 28.338 | 13.420 | -6.858 | 1.00 | 23.02 |
| 8928 | C | LEU | B | 308 | 27.651 | 14.663 | -11.058 | 1.00 | 22.32 |
| 8929 | O | LEU | B | 308 | 27.411 | 15.858 | -10.863 | 1.00 | 21.59 |
| 8930 | N | GLU | B | 309 | 27.861 | 14.144 | -12.270 | 1.00 | 22.83 |
| 8932 | CA | GLU | B | 309 | 27.716 | 14.933 | -13.480 | 1.00 | 23.58 |
| 8934 | CB | GLU | B | 309 | 28.227 | 14.192 | -14.720 | 1.00 | 24.19 |
| 8937 | CG | GLU | B | 309 | 29.708 | 13.867 | -14.789 | 1.00 | 27.75 |
| 8940 | CD | GLU | B | 309 | 30.025 | 12.941 | -15.962 | 1.00 | 31.36 |
| 8941 | OE1 | GLU | B | 309 | 29.515 | 13.205 | -17.070 | 1.00 | 34.68 |
| 8942 | OE2 | GLU | B | 309 | 30.758 | 11.938 | -15.784 | 1.00 | 33.57 |
| 8943 | C | GLU | B | 309 | 26.241 | 15.247 | -13.705 | 1.00 | 23.21 |
| 8944 | O | GLU | B | 309 | 25.897 | 16.382 | -14.000 | 1.00 | 23.30 |
| 8945 | N | ALA | B | 310 | 25.378 | 14.238 | -13.592 | 1.00 | 22.93 |
| 8947 | CA | ALA | B | 310 | 23.954 | 14.418 | -13.865 | 1.00 | 23.17 |
| 8949 | CB | ALA | B | 310 | 23.219 | 13.063 | -13.846 | 1.00 | 23.72 |
| 8953 | C | ALA | B | 310 | 23.348 | 15.383 | -12.844 | 1.00 | 22.99 |
| 8954 | O | ALA | B | 310 | 22.530 | 16.240 | -13.186 | 1.00 | 22.84 |
| 8955 | N | LEU | B | 311 | 23.786 | 15.250 | -11.596 | 1.00 | 22.47 |
| 8957 | CA | LEU | B | 311 | 23.331 | 16.111 | -10.518 | 1.00 | 22.39 |
| 8959 | CB | LEU | B | 311 | 23.841 | 15.623 | -9.166 | 1.00 | 22.42 |
| 8962 | CG | LEU | B | 311 | 23.319 | 16.420 | -7.973 | 1.00 | 23.49 |
| 8964 | CD1 | LEU | B | 311 | 21.813 | 16.473 | -7.938 | 1.00 | 26.09 |
| 8968 | CD2 | LEU | B | 311 | 23.835 | 15.859 | -6.701 | 1.00 | 25.91 |
| 8972 | C | LEU | B | 311 | 23.766 | 17.540 | -10.732 | 1.00 | 21.68 |
| 8973 | O | LEU | B | 311 | 22.993 | 18.452 | -10.511 | 1.00 | 21.68 |
| 8974 | N | ALA | B | 312 | 25.002 | 17.742 | -11.173 | 1.00 | 21.62 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 8976 | CA | ALA | B | 312 | 25.507 | 19.094 | -11.401 | 1.00 | 21.18 |
| 8978 | CB | ALA | B | 312 | 26.970 | 19.055 | -11.829 | 1.00 | 20.99 |
| 8982 | C | ALA | B | 312 | 24.649 | 19.827 | -12.437 | 1.00 | 21.29 |
| 8983 | O | ALA | B | 312 | 24.260 | 20.978 | -12.221 | 1.00 | 20.84 |
| 8984 | N | ASP | B | 313 | 24.356 | 19.157 | -13.557 | 1.00 | 21.52 |
| 8986 | CA | ASP | B | 313 | 23.462 | 19.700 | -14.575 | 1.00 | 21.89 |
| 8988 | CB | ASP | B | 313 | 23.298 | 18.717 | -15.749 | 1.00 | 22.19 |
| 8991 | CG | ASP | B | 313 | 24.484 | 18.721 | -16.695 | 1.00 | 24.91 |
| 8992 | OD1 | ASP | B | 313 | 25.217 | 19.734 | -16.774 | 1.00 | 27.76 |
| 8993 | OD2 | ASP | B | 313 | 24.754 | 17.744 | -17.418 | 1.00 | 28.49 |
| 8994 | C | ASP | B | 313 | 22.091 | 19.989 | -13.985 | 1.00 | 21.17 |
| 8995 | O | ASP | B | 313 | 21.517 | 21.065 | -14.199 | 1.00 | 21.04 |
| 8996 | N | TYR | B | 314 | 21.566 | 19.037 | -13.226 | 1.00 | 20.68 |
| 8998 | CA | TYR | B | 314 | 20.230 | 19.196 | -12.667 | 1.00 | 21.00 |
| 9000 | CB | TYR | B | 314 | 19.804 | 17.946 | -11.921 | 1.00 | 20.75 |
| 9003 | CG | TYR | B | 314 | 18.419 | 18.039 | -11.344 | 1.00 | 21.19 |
| 9004 | CD1 | TYR | B | 314 | 18.220 | 18.052 | -9.966 | 1.00 | 20.91 |
| 9006 | CE1 | TYR | B | 314 | 16.956 | 18.127 | -9.432 | 1.00 | 21.89 |
| 9008 | CZ | TYR | B | 314 | 15.853 | 18.187 | -10.268 | 1.00 | 24.30 |
| 9009 | OH | TYR | B | 314 | 14.587 | 18.254 | -9.704 | 1.00 | 26.37 |
| 9011 | CE2 | TYR | B | 314 | 16.020 | 18.192 | -11.643 | 1.00 | 23.04 |
| 9013 | CD2 | TYR | B | 314 | 17.299 | 18.112 | -12.174 | 1.00 | 22.71 |
| 9015 | C | TYR | B | 314 | 20.145 | 20.397 | -11.726 | 1.00 | 21.05 |
| 9016 | O | TYR | B | 314 | 19.109 | 21.018 | -11.613 | 1.00 | 20.68 |
| 9017 | N | ILE | B | 315 | 21.239 | 20.713 | -11.043 | 1.00 | 21.13 |
| 9019 | CA | ILE | B | 315 | 21.245 | 21.825 | -10.102 | 1.00 | 21.51 |
| 9021 | CB | ILE | B | 315 | 22.635 | 21.881 | -9.382 | 1.00 | 21.42 |
| 9023 | CG1 | ILE | B | 315 | 22.663 | 20.817 | -8.279 | 1.00 | 21.51 |
| 9026 | CD1 | ILE | B | 315 | 24.007 | 20.664 | -7.593 | 1.00 | 22.06 |
| 9030 | CG2 | ILE | B | 315 | 22.891 | 23.256 | -8.766 | 1.00 | 22.35 |
| 9034 | C | ILE | B | 315 | 20.874 | 23.159 | -10.774 | 1.00 | 21.80 |
| 9035 | O | ILE | B | 315 | 20.237 | 24.017 | -10.162 | 1.00 | 21.41 |
| 9036 | N | ILE | B | 316 | 21.245 | 23.328 | -12.041 | 1.00 | 22.74 |
| 9038 | CA | ILE | B | 316 | 20.886 | 24.542 | -12.765 | 1.00 | 23.55 |
| 9040 | CB | ILE | B | 316 | 22.148 | 25.209 | -13.364 | 1.00 | 23.89 |
| 9042 | CG1 | ILE | B | 316 | 22.714 | 24.400 | -14.540 | 1.00 | 24.25 |
| 9045 | CD1 | ILE | B | 316 | 23.776 | 25.141 | -15.342 | 1.00 | 24.35 |
| 9049 | CG2 | ILE | B | 316 | 23.190 | 25.406 | -12.269 | 1.00 | 24.66 |
| 9053 | C | ILE | B | 316 | 19.799 | 24.344 | -13.828 | 1.00 | 23.85 |
| 9054 | O | ILE | B | 316 | 19.400 | 25.315 | -14.470 | 1.00 | 24.70 |
| 9055 | N | GLN | B | 317 | 19.319 | 23.110 | -14.015 | 1.00 | 23.74 |
| 9057 | CA | GLN | B | 317 | 18.251 | 22.833 | -14.990 | 1.00 | 23.91 |
| 9059 | CB | GLN | B | 317 | 18.584 | 21.602 | -15.821 | 1.00 | 24.17 |
| 9062 | CG | GLN | B | 317 | 19.713 | 21.884 | -16.815 | 1.00 | 26.77 |
| 9065 | CD | GLN | B | 317 | 20.172 | 20.670 | -17.588 | 1.00 | 28.31 |
| 9066 | OE1 | GLN | B | 317 | 21.115 | 20.760 | -18.367 | 1.00 | 33.64 |
| 9067 | NE2 | GLN | B | 317 | 19.520 | 19.540 | -17.382 | 1.00 | 32.21 |
| 9070 | C | GLN | B | 317 | 16.887 | 22.687 | -14.329 | 1.00 | 23.46 |
| 9071 | O | GLN | B | 317 | 15.857 | 22.873 | -14.981 | 1.00 | 23.30 |
| 9072 | N | ARG | B | 318 | 16.889 | 22.369 | -13.033 | 1.00 | 23.14 |
| 9074 | CA | ARG | B | 318 | 15.666 | 22.175 | -12.249 | 1.00 | 22.83 |
| 9076 | CB | ARG | B | 318 | 16.010 | 21.784 | -10.806 | 1.00 | 22.67 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 9079 | CG | ARG | B | 318 | 16.722 | 22.887 | -10.002 | 1.00 | 21.91 |
| 9082 | CD | ARG | B | 318 | 17.584 | 22.348 | -8.871 | 1.00 | 20.80 |
| 9085 | NE | ARG | B | 318 | 18.319 | 23.405 | -8.180 | 1.00 | 19.32 |
| 9087 | CZ | ARG | B | 318 | 17.807 | 24.145 | -7.212 | 1.00 | 19.88 |
| 9088 | NH1 | ARG | B | 318 | 18.559 | 25.083 | -6.640 | 1.00 | 20.86 |
| 9091 | NH2 | ARG | B | 318 | 16.547 | 23.956 | -6.806 | 1.00 | 18.83 |
| 9094 | C | ARG | B | 318 | 14.826 | 23.434 | -12.199 | 1.00 | 23.29 |
| 9095 | O | ARG | B | 318 | 15.361 | 24.542 | -12.222 | 1.00 | 22.52 |
| 9096 | N | ASN | B | 319 | 13.513 | 23.232 | -12.116 | 1.00 | 24.23 |
| 9098 | CA | ASN | B | 319 | 12.519 | 24.294 | -11.967 | 1.00 | 25.30 |
| 9100 | CB | ASN | B | 319 | 11.404 | 24.132 | -13.023 | 1.00 | 25.73 |
| 9103 | CG | ASN | B | 319 | 10.586 | 22.855 | -12.843 | 1.00 | 27.06 |
| 9104 | OD1 | ASN | B | 319 | 10.893 | 22.015 | -12.003 | 1.00 | 30.28 |
| 9105 | ND2 | ASN | B | 319 | 9.526 | 22.712 | -13.642 | 1.00 | 30.33 |
| 9108 | C | ASN | B | 319 | 11.922 | 24.303 | -10.550 | 1.00 | 26.15 |
| 9109 | O | ASN | B | 319 | 10.931 | 24.991 | -10.282 | 1.00 | 26.07 |
| 9110 | N | LYS | B | 320 | 12.523 | 23.510 | -9.663 | 1.00 | 26.76 |
| 9112 | CA | LYS | B | 320 | 12.057 | 23.349 | -8.295 | 1.00 | 27.55 |
| 9114 | CB | LYS | B | 320 | 10.997 | 22.245 | -8.214 | 1.00 | 28.24 |
| 9117 | CG | LYS | B | 320 | 11.437 | 20.876 | -8.748 | 1.00 | 30.42 |
| 9120 | CD | LYS | B | 320 | 10.388 | 19.777 | -8.483 | 1.00 | 34.02 |
| 9123 | CE | LYS | B | 320 | 9.281 | 19.733 | -9.557 | 1.00 | 35.81 |
| 9126 | NZ | LYS | B | 320 | 9.763 | 19.297 | -10.914 | 1.00 | 37.55 |
| 9130 | C | LYS | B | 320 | 13.212 | 23.017 | -7.370 | 1.00 | 27.53 |
| 9131 | O | LYS | B | 320 | 13.045 | 23.018 | -6.148 | 1.00 | 27.94 |
| 9132 | OXT | LYS | B | 320 | 14.311 | 22.729 | -7.848 | 1.00 | 26.55 |
| 9133 | O9 | ipp | X | 900 | 59.879 | 67.784 | 6.844 | 1.00 | 22.62 |
| 9134 | P7 | ipp | X | 900 | 60.281 | 67.030 | 8.078 | 1.00 | 20.44 |
| 9135 | O8 | ipp | X | 900 | 61.128 | 65.793 | 7.905 | 1.00 | 20.16 |
| 9136 | O10 | ipp | X | 900 | 58.921 | 66.747 | 8.923 | 1.00 | 20.32 |
| 9137 | P11 | ipp | X | 900 | 58.096 | 65.364 | 9.039 | 1.00 | 20.72 |
| 9138 | O13 | ipp | X | 900 | 58.271 | 64.667 | 7.712 | 1.00 | 21.48 |
| 9139 | O12 | ipp | X | 900 | 58.760 | 64.598 | 10.167 | 1.00 | 20.42 |
| 9140 | O14 | ipp | X | 900 | 56.677 | 65.719 | 9.388 | 1.00 | 19.87 |
| 9141 | O6 | ipp | X | 900 | 61.085 | 68.067 | 9.000 | 1.00 | 23.40 |
| 9142 | C5 | ipp | X | 900 | 60.446 | 69.278 | 9.396 | 1.00 | 22.55 |
| 9145 | C4 | ipp | X | 900 | 61.386 | 70.077 | 10.277 | 1.00 | 23.87 |
| 9148 | C2 | ipp | X | 900 | 62.729 | 70.303 | 9.627 | 1.00 | 24.00 |
| 9149 | C3 | ipp | X | 900 | 62.847 | 70.872 | 8.237 | 1.00 | 23.48 |
| 9153 | C1 | ipp | X | 900 | 63.818 | 70.021 | 10.311 | 1.00 | 24.77 |
| 9156 | O12 | ris | X | 901 | 57.820 | 74.304 | 11.572 | 1.00 | 21.28 |
| 9157 | P9 | ris | X | 901 | 58.623 | 73.691 | 10.433 | 1.00 | 21.35 |
| 9158 | O11 | ris | X | 901 | 58.329 | 74.511 | 8.992 | 1.00 | 22.29 |
| 9160 | O10 | ris | X | 901 | 58.206 | 72.094 | 10.263 | 1.00 | 22.10 |
| 9162 | C8 | ris | X | 901 | 60.334 | 73.798 | 10.791 | 1.00 | 20.58 |
| 9163 | O13 | ris | X | 901 | 61.051 | 73.167 | 9.710 | 1.00 | 21.47 |
| 9165 | P14 | ris | X | 901 | 60.832 | 75.467 | 10.955 | 1.00 | 21.49 |
| 9166 | O16 | ris | X | 901 | 60.487 | 76.175 | 9.664 | 1.00 | 20.67 |
| 9167 | O15 | ris | X | 901 | 60.014 | 76.127 | 12.259 | 1.00 | 20.29 |
| 9169 | O17 | ris | X | 901 | 62.473 | 75.654 | 11.235 | 1.00 | 16.79 |
| 9171 | C7 | ris | X | 901 | 60.517 | 73.036 | 12.110 | 1.00 | 20.01 |
| 9174 | C2 | ris | X | 901 | 61.916 | 72.843 | 12.658 | 1.00 | 20.04 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 9175 | C1 | ris | X | 901 | 62.030 | 72.693 | 14.038 | 1.00 | 22.23 |
| 9177 | C6 | ris | X | 901 | 63.284 | 72.496 | 14.614 | 1.00 | 21.92 |
| 9179 | C5 | ris | X | 901 | 64.396 | 72.454 | 13.790 | 1.00 | 21.90 |
| 9181 | N4 | ris | X | 901 | 64.272 | 72.597 | 12.461 | 1.00 | 20.50 |
| 9182 | C3 | ris | X | 901 | 63.073 | 72.787 | 11.887 | 1.00 | 20.38 |
| 9184 | O9 | ipp | X | 902 | 16.064 | 23.295 | -2.975 | 1.00 | 21.48 |
| 9185 | P7 | ipp | X | 902 | 16.496 | 22.587 | -1.731 | 1.00 | 20.32 |
| 9186 | O8 | ipp | X | 902 | 17.402 | 21.368 | -1.817 | 1.00 | 20.60 |
| 9187 | O10 | ipp | X | 902 | 15.180 | 22.297 | -0.852 | 1.00 | 19.29 |
| 9188 | P11 | ipp | X | 902 | 14.357 | 20.933 | -0.731 | 1.00 | 21.41 |
| 9189 | O13 | ipp | X | 902 | 14.501 | 20.303 | -2.099 | 1.00 | 21.14 |
| 9190 | O12 | ipp | X | 902 | 15.018 | 20.139 | 0.361 | 1.00 | 19.56 |
| 9191 | O14 | ipp | X | 902 | 12.943 | 21.318 | -0.386 | 1.00 | 20.18 |
| 9192 | O6 | ipp | X | 902 | 17.282 | 23.658 | -0.828 | 1.00 | 21.57 |
| 9193 | C5 | ipp | X | 902 | 16.665 | 24.901 | -0.520 | 1.00 | 20.59 |
| 9196 | C4 | ipp | X | 902 | 17.539 | 25.684 | 0.451 | 1.00 | 20.72 |
| 9199 | C2 | ipp | X | 902 | 18.923 | 25.954 | -0.086 | 1.00 | 20.12 |
| 9200 | C3 | ipp | X | 902 | 19.094 | 26.613 | -1.425 | 1.00 | 20.10 |
| 9204 | C1 | ipp | X | 902 | 19.970 | 25.641 | 0.637 | 1.00 | 19.72 |
| 9207 | O12 | ris | X | 903 | 13.949 | 29.944 | 1.653 | 1.00 | 18.96 |
| 9208 | P9 | ris | X | 903 | 14.827 | 29.319 | 0.595 | 1.00 | 18.15 |
| 9209 | O11 | ris | X | 903 | 14.564 | 30.066 | -0.891 | 1.00 | 17.76 |
| 9211 | O10 | ris | X | 903 | 14.479 | 27.699 | 0.371 | 1.00 | 17.12 |
| 9213 | C8 | ris | X | 903 | 16.543 | 29.484 | 1.000 | 1.00 | 16.83 |
| 9214 | O13 | ris | X | 903 | 17.268 | 28.905 | -0.099 | 1.00 | 14.71 |
| 9216 | P14 | ris | X | 903 | 17.105 | 31.143 | 1.147 | 1.00 | 16.07 |
| 9217 | O16 | ris | X | 903 | 16.424 | 31.703 | 2.361 | 1.00 | 18.08 |
| 9218 | O15 | ris | X | 903 | 18.754 | 31.239 | 1.421 | 1.00 | 20.15 |
| 9220 | O17 | ris | X | 903 | 16.681 | 31.883 | -0.303 | 1.00 | 17.24 |
| 9222 | C7 | ris | X | 903 | 16.736 | 28.711 | 2.310 | 1.00 | 15.64 |
| 9225 | C2 | ris | X | 903 | 18.144 | 28.461 | 2.843 | 1.00 | 17.89 |
| 9226 | C1 | ris | X | 903 | 18.231 | 28.146 | 4.193 | 1.00 | 17.51 |
| 9228 | C6 | ris | X | 903 | 19.477 | 27.908 | 4.776 | 1.00 | 17.87 |
| 9230 | C5 | ris | X | 903 | 20.612 | 27.985 | 3.980 | 1.00 | 18.68 |
| 9232 | N4 | ris | X | 903 | 20.535 | 28.281 | 2.665 | 1.00 | 18.45 |
| 9233 | C3 | ris | X | 903 | 19.332 | 28.506 | 2.084 | 1.00 | 18.77 |
| 9235 | MG | MG | X | 904 | 15.574 | 31.310 | -1.873 | 1.00 | 21.07 |
| 9236 | MG | MG | X | 905 | 17.080 | 32.751 | 3.968 | 1.00 | 17.94 |
| 9237 | MG | MG | X | 906 | 14.279 | 31.564 | 2.944 | 1.00 | 18.98 |
| 9238 | MG | MG | X | 907 | 58.027 | 75.928 | 12.811 | 1.00 | 21.97 |
| 9239 | MG | MG | X | 908 | 59.508 | 75.731 | 8.080 | 1.00 | 25.32 |
| 9240 | MG | MG | X | 909 | 60.807 | 77.116 | 13.792 | 1.00 | 19.86 |
| 9241 | OW0 | HOH | X | 1 | 69.581 | 70.101 | 13.536 | 1.00 | 18.91 |
| 9244 | OW0 | HOH | X | 2 | 62.678 | 62.339 | 10.204 | 1.00 | 15.42 |
| 9247 | OW0 | HOH | X | 3 | 25.799 | 25.747 | 3.926 | 1.00 | 15.73 |
| 9250 | OW0 | HOH | X | 4 | 59.333 | 62.010 | 10.213 | 1.00 | 18.17 |
| 9253 | OW0 | HOH | X | 5 | 18.822 | 17.964 | 0.386 | 1.00 | 18.32 |
| 9256 | OW0 | HOH | X | 6 | 13.596 | 24.842 | -2.548 | 1.00 | 13.98 |
| 9259 | OW0 | HOH | X | 7 | 60.443 | 70.120 | 5.487 | 1.00 | 20.05 |
| 9262 | OW0 | HOH | X | 8 | 67.024 | 68.022 | 10.947 | 1.00 | 18.31 |
| 9265 | OW0 | HOH | X | 9 | 75.891 | 66.532 | 13.529 | 1.00 | 16.24 |
| 9268 | OW0 | HOH | X | 10 | 61.389 | 59.407 | 28.540 | 1.00 | 15.76 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 9271 | OW0 | HOH | X | 11 | 16.713 | 25.479 | -4.403 | 1.00 | 16.69 |
| 9274 | OW0 | HOH | X | 12 | 17.228 | 19.008 | -1.948 | 1.00 | 17.97 |
| 9277 | OW0 | HOH | X | 13 | 60.948 | 63.338 | 7.816 | 1.00 | 17.21 |
| 9280 | OW0 | HOH | X | 14 | 12.537 | 21.690 | 6.873 | 1.00 | 20.29 |
| 9283 | OW0 | HOH | X | 15 | 17.395 | 34.432 | 2.680 | 1.00 | 15.95 |
| 9286 | OW0 | HOH | X | 16 | 22.715 | 24.983 | 3.509 | 1.00 | 21.00 |
| 9289 | OW0 | HOH | X | 17 | 23.103 | 23.679 | 1.175 | 1.00 | 16.66 |
| 9292 | OW0 | HOH | X | 18 | 60.488 | 77.235 | 6.934 | 1.00 | 16.27 |
| 9295 | OW0 | HOH | X | 19 | 57.327 | 69.233 | 7.233 | 1.00 | 17.06 |
| 9298 | OW0 | HOH | X | 20 | 15.505 | 17.649 | 0.655 | 1.00 | 17.89 |
| 9301 | OW0 | HOH | X | 21 | 34.673 | 22.728 | -9.839 | 1.00 | 22.21 |
| 9304 | OW0 | HOH | X | 22 | 12.191 | 23.940 | -0.324 | 1.00 | 14.99 |
| 9307 | OW0 | HOH | X | 23 | 4.461 | 26.280 | 19.031 | 1.00 | 23.20 |
| 9310 | OW0 | HOH | X | 24 | 72.420 | 88.509 | 2.009 | 1.00 | 28.92 |
| 9313 | OW0 | HOH | X | 25 | 73.365 | 71.690 | 24.882 | 1.00 | 15.83 |
| 9316 | OW0 | HOH | X | 26 | 9.311 | 27.134 | 10.014 | 1.00 | 16.86 |
| 9319 | OW0 | HOH | X | 27 | 33.303 | 4.388 | 14.111 | 1.00 | 23.61 |
| 9322 | OW0 | HOH | X | 28 | 9.972 | 29.039 | 2.416 | 1.00 | 19.40 |
| 9325 | OW0 | HOH | X | 29 | 20.315 | 24.167 | 4.178 | 1.00 | 21.86 |
| 9328 | OW0 | HOH | X | 30 | 23.161 | 10.579 | 20.659 | 1.00 | 23.73 |
| 9331 | OW0 | HOH | X | 31 | 62.889 | 76.521 | 13.608 | 1.00 | 18.10 |
| 9334 | OW0 | HOH | X | 32 | 14.368 | 17.510 | 4.944 | 1.00 | 24.43 |
| 9337 | OW0 | HOH | X | 33 | 31.222 | 26.334 | 11.934 | 1.00 | 21.87 |
| 9340 | OW0 | HOH | X | 34 | 17.123 | 34.428 | -0.050 | 1.00 | 18.82 |
| 9343 | OW0 | HOH | X | 35 | 65.244 | 84.346 | -6.827 | 1.00 | 23.12 |
| 9346 | OW0 | HOH | X | 36 | 53.273 | 71.292 | 19.938 | 1.00 | 20.38 |
| 9349 | OW0 | HOH | X | 37 | 75.108 | 70.654 | 21.698 | 1.00 | 19.01 |
| 9352 | OW0 | HOH | X | 38 | 61.370 | 78.383 | 15.450 | 1.00 | 24.45 |
| 9355 | OW0 | HOH | X | 39 | 64.170 | 68.585 | 13.753 | 1.00 | 23.11 |
| 9358 | OW0 | HOH | X | 40 | 15.187 | 3.524 | -3.226 | 1.00 | 21.48 |
| 9361 | OW0 | HOH | X | 41 | 20.358 | 39.276 | 1.884 | 1.00 | 22.25 |
| 9364 | OW0 | HOH | X | 42 | 59.729 | 80.370 | 3.839 | 1.00 | 25.41 |
| 9367 | OW0 | HOH | X | 43 | 9.394 | 25.625 | 7.660 | 1.00 | 19.98 |
| 9370 | OW0 | HOH | X | 44 | 19.279 | 13.591 | 19.445 | 1.00 | 25.74 |
| 9373 | OW0 | HOH | X | 45 | 18.592 | 28.894 | 9.372 | 1.00 | 21.52 |
| 9376 | OW0 | HOH | X | 46 | 16.733 | 32.742 | -2.993 | 1.00 | 17.70 |
| 9379 | OW0 | HOH | X | 47 | 28.337 | 35.553 | 9.793 | 1.00 | 24.55 |
| 9382 | OW0 | HOH | X | 48 | 71.766 | 52.024 | 1.660 | 1.00 | 25.10 |
| 9385 | OW0 | HOH | X | 49 | 5.509 | 18.812 | 21.857 | 1.00 | 25.11 |
| 9388 | OW0 | HOH | X | 50 | 25.249 | 44.467 | -11.635 | 1.00 | 22.90 |
| 9391 | OW0 | HOH | X | 51 | 16.089 | 35.932 | -5.867 | 1.00 | 20.15 |
| 9394 | OW0 | HOH | X | 52 | 50.870 | 75.101 | 10.886 | 1.00 | 22.51 |
| 9397 | OW0 | HOH | X | 53 | 58.111 | 59.051 | 3.773 | 1.00 | 23.52 |
| 9400 | OW0 | HOH | X | 54 | 84.343 | 49.350 | 23.069 | 1.00 | 19.58 |
| 9403 | OW0 | HOH | X | 55 | 56.087 | 75.553 | 13.615 | 1.00 | 15.17 |
| 9406 | OW0 | HOH | X | 56 | 19.494 | 34.654 | -1.382 | 1.00 | 20.86 |
| 9409 | OW0 | HOH | X | 57 | 8.799 | 19.400 | 4.773 | 1.00 | 21.44 |
| 9412 | OW0 | HOH | X | 58 | 39.726 | 12.512 | 12.694 | 1.00 | 37.61 |
| 9415 | OW0 | HOH | X | 59 | 12.786 | 3.396 | 7.777 | 1.00 | 28.21 |
| 9418 | OW0 | HOH | X | 61 | 33.547 | 28.085 | -16.167 | 1.00 | 24.17 |
| 9421 | OW0 | HOH | X | 62 | 60.548 | 68.421 | 32.431 | 1.00 | 22.66 |
| 9424 | OW0 | HOH | X | 63 | 52.652 | 63.594 | 14.580 | 1.00 | 21.16 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 9427 | OW0 | HOH | X | 64 | 63.267 | 78.956 | 8.228 | 1.00 | 23.96 |
| 9430 | OW0 | HOH | X | 65 | 21.674 | 40.154 | -16.591 | 1.00 | 19.82 |
| 9433 | OW0 | HOH | X | 66 | 62.524 | 73.265 | 19.235 | 1.00 | 24.72 |
| 9436 | OW0 | HOH | X | 67 | 50.175 | 67.476 | 14.681 | 1.00 | 24.07 |
| 9439 | OW0 | HOH | X | 68 | 16.317 | 24.542 | 22.592 | 1.00 | 24.88 |
| 9442 | OW0 | HOH | X | 70 | 13.596 | 32.913 | 1.425 | 1.00 | 18.95 |
| 9445 | OW0 | HOH | X | 71 | 33.743 | 4.683 | -9.292 | 1.00 | 21.88 |
| 9448 | OW0 | HOH | X | 72 | 84.877 | 52.105 | 15.691 | 1.00 | 35.89 |
| 9451 | OW0 | HOH | X | 73 | 28.069 | 7.721 | -7.921 | 1.00 | 22.28 |
| 9454 | OW0 | HOH | X | 74 | 29.256 | 1.053 | 13.166 | 1.00 | 28.61 |
| 9457 | OW0 | HOH | X | 75 | 26.790 | -1.137 | 5.597 | 1.00 | 33.71 |
| 9460 | OW0 | HOH | X | 76 | 33.840 | 27.398 | -6.991 | 1.00 | 26.70 |
| 9463 | OW0 | HOH | X | 77 | 20.039 | 38.545 | -21.843 | 1.00 | 59.27 |
| 9466 | OW0 | HOH | X | 78 | 49.910 | 55.142 | 25.447 | 1.00 | 26.46 |
| 9469 | OW0 | HOH | X | 79 | 9.843 | 14.477 | -1.615 | 1.00 | 27.96 |
| 9472 | OW0 | HOH | X | 80 | 36.808 | 16.350 | 8.648 | 1.00 | 22.19 |
| 9475 | OW0 | HOH | X | 81 | 43.245 | 14.999 | 0.753 | 1.00 | 22.13 |
| 9478 | OW0 | HOH | X | 82 | 57.361 | 79.956 | 11.239 | 1.00 | 25.78 |
| 9481 | OW0 | HOH | X | 83 | 9.775 | 24.342 | -1.506 | 1.00 | 22.49 |
| 9484 | OW0 | HOH | X | 84 | 68.131 | 69.501 | 22.346 | 1.00 | 28.17 |
| 9487 | OW0 | HOH | X | 85 | 64.173 | 83.689 | 11.530 | 1.00 | 19.53 |
| 9490 | OW0 | HOH | X | 86 | 58.920 | 48.042 | 6.438 | 1.00 | 22.32 |
| 9493 | OW0 | HOH | X | 87 | 57.493 | 77.168 | 11.232 | 1.00 | 19.16 |
| 9496 | OW0 | HOH | X | 88 | 77.326 | 71.627 | 2.643 | 1.00 | 27.72 |
| 9499 | OW0 | HOH | X | 89 | 74.547 | 71.580 | 7.451 | 1.00 | 24.66 |
| 9502 | OW0 | HOH | X | 91 | 48.469 | 59.380 | 21.046 | 1.00 | 23.24 |
| 9505 | OW0 | HOH | X | 92 | 59.723 | 83.049 | 3.647 | 1.00 | 26.08 |
| 9508 | OW0 | HOH | X | 93 | 29.853 | 24.288 | -1.800 | 1.00 | 33.40 |
| 9511 | O | HOH | X | 94 | 56.128 | 56.547 | -0.069 | 1.00 | 31.76 |
| 9514 | O | HOH | X | 95 | 60.992 | 57.155 | 5.055 | 1.00 | 25.17 |
| 9517 | O | HOH | X | 96 | 57.412 | 60.876 | 1.767 | 1.00 | 27.49 |
| 9520 | O | HOH | X | 98 | 10.425 | 34.341 | 14.720 | 1.00 | 25.28 |
| 9523 | O | HOH | X | 99 | 58.393 | 61.924 | 14.465 | 1.00 | 21.57 |
| 9526 | O | HOH | X | 100 | 15.514 | 40.203 | -8.447 | 1.00 | 25.83 |
| 9529 | O | HOH | X | 101 | 71.395 | 44.872 | 6.706 | 1.00 | 23.21 |
| 9532 | O | HOH | X | 102 | 59.088 | 84.453 | 1.416 | 1.00 | 21.13 |
| 9535 | O | HOH | X | 103 | 10.805 | 35.476 | 2.484 | 1.00 | 30.21 |
| 9538 | O | HOH | X | 104 | 78.675 | 67.094 | -0.168 | 1.00 | 30.94 |
| 9541 | O | HOH | X | 105 | 53.216 | 69.834 | 17.573 | 1.00 | 21.88 |
| 9544 | O | HOH | X | 106 | 11.540 | 21.193 | -2.775 | 1.00 | 23.63 |
| 9547 | O | HOH | X | 107 | 56.434 | 66.036 | 16.603 | 1.00 | 21.18 |
| 9550 | O | HOH | X | 108 | 53.589 | 69.002 | 8.469 | 1.00 | 26.03 |
| 9553 | O | HOH | X | 109 | 22.171 | 2.588 | 12.364 | 1.00 | 25.07 |
| 9556 | O | HOH | X | 110 | 77.332 | 49.094 | 0.357 | 1.00 | 25.35 |
| 9559 | O | HOH | X | 111 | 33.771 | 36.319 | -2.063 | 1.00 | 30.82 |
| 9562 | O | HOH | X | 112 | 12.214 | 37.251 | -5.519 | 1.00 | 20.62 |
| 9565 | O | HOH | X | 113 | 68.012 | 47.978 | 18.112 | 1.00 | 22.53 |
| 9568 | O | HOH | X | 114 | 52.583 | 66.344 | 14.741 | 1.00 | 24.60 |
| 9571 | O | HOH | X | 115 | 54.317 | 78.524 | 24.510 | 1.00 | 28.76 |
| 9574 | O | HOH | X | 116 | 17.315 | 3.665 | 4.180 | 1.00 | 31.96 |
| 9577 | O | HOH | X | 117 | 41.900 | 14.903 | -5.570 | 1.00 | 23.73 |
| 9580 | O | HOH | X | 118 | 25.232 | 6.606 | -7.167 | 1.00 | 24.37 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 9583 | O | HOH | X | 119 | 69.198 | 51.022 | 2.442 | 1.00 | 32.30 |
| 9586 | O | HOH | X | 120 | 54.454 | 75.970 | 7.898 | 1.00 | 29.61 |
| 9589 | O | HOH | X | 121 | 72.835 | 54.092 | -0.028 | 1.00 | 28.37 |
| 9592 | O | HOH | X | 122 | 13.624 | 16.407 | -7.904 | 1.00 | 26.27 |
| 9595 | O | HOH | X | 123 | 52.606 | 51.548 | 23.966 | 1.00 | 31.75 |
| 9598 | O | HOH | X | 124 | 64.545 | 60.261 | -5.452 | 1.00 | 26.24 |
| 9601 | O | HOH | X | 125 | 48.485 | 73.411 | 29.403 | 1.00 | 35.53 |
| 9604 | O | HOH | X | 126 | 73.394 | 45.286 | 22.697 | 1.00 | 31.73 |
| 9607 | O | HOH | X | 127 | 1.619 | 16.387 | 23.748 | 1.00 | 35.87 |
| 9610 | O | HOH | X | 128 | 51.331 | 52.037 | 31.882 | 1.00 | 32.80 |
| 9613 | O | HOH | X | 130 | 59.702 | 84.785 | 5.880 | 1.00 | 28.09 |
| 9616 | O | HOH | X | 131 | 35.875 | 32.733 | -2.230 | 1.00 | 41.90 |
| 9619 | O | HOH | X | 132 | 56.078 | 68.294 | 9.410 | 1.00 | 23.25 |
| 9622 | O | HOH | X | 133 | 68.940 | 88.925 | -1.936 | 1.00 | 24.65 |
| 9625 | O | HOH | X | 134 | 66.234 | 47.041 | 21.983 | 1.00 | 27.75 |
| 9628 | O | HOH | X | 135 | 61.333 | 46.476 | 6.833 | 1.00 | 25.98 |
| 9631 | O | HOH | X | 136 | 67.556 | 54.792 | 30.084 | 1.00 | 27.45 |
| 9634 | O | HOH | X | 137 | 40.092 | 4.846 | 14.202 | 1.00 | 33.56 |
| 9637 | O | HOH | X | 138 | 6.434 | 23.324 | 4.635 | 1.00 | 23.23 |
| 9640 | O | HOH | X | 139 | 53.326 | 52.199 | 10.569 | 1.00 | 27.46 |
| 9643 | O | HOH | X | 140 | 16.797 | 40.699 | -15.388 | 1.00 | 31.25 |
| 9646 | O | HOH | X | 141 | 55.505 | 68.569 | 5.472 | 1.00 | 31.05 |
| 9649 | O | HOH | X | 142 | 19.829 | 28.141 | -14.550 | 1.00 | 32.03 |
| 9652 | O | HOH | X | 143 | 72.192 | 80.036 | 19.386 | 1.00 | 26.69 |
| 9655 | O | HOH | X | 144 | 49.567 | 62.818 | 10.675 | 1.00 | 36.36 |
| 9658 | O | HOH | X | 145 | 77.624 | 80.795 | 7.572 | 1.00 | 30.84 |
| 9661 | O | HOH | X | 146 | 70.251 | 84.697 | 14.333 | 1.00 | 29.10 |
| 9664 | O | HOH | X | 147 | 22.147 | 28.439 | -15.860 | 1.00 | 25.06 |
| 9667 | O | HOH | X | 149 | 13.634 | 35.572 | 1.265 | 1.00 | 25.62 |
| 9670 | O | HOH | X | 150 | 82.244 | 46.629 | 23.769 | 1.00 | 35.68 |
| 9673 | O | HOH | X | 151 | 63.846 | 88.990 | 3.561 | 1.00 | 28.36 |
| 9676 | O | HOH | X | 152 | 64.405 | 73.293 | -9.004 | 1.00 | 59.74 |
| 9679 | O | HOH | X | 153 | 19.585 | 44.233 | -0.968 | 1.00 | 31.22 |
| 9682 | O | HOH | X | 154 | 17.128 | 12.637 | -4.589 | 1.00 | 25.38 |
| 9685 | O | HOH | X | 155 | 5.113 | 33.908 | 7.713 | 1.00 | 38.08 |
| 9688 | O | HOH | X | 156 | 30.306 | 34.937 | -7.899 | 1.00 | 34.44 |
| 9691 | O | HOH | X | 157 | 3.129 | 22.986 | -4.541 | 1.00 | 39.21 |
| 9694 | O | HOH | X | 158 | 66.626 | 69.399 | 13.372 | 1.00 | 23.00 |
| 9697 | O | HOH | X | 159 | 63.446 | 57.641 | 29.205 | 1.00 | 27.23 |
| 9700 | O | HOH | X | 160 | 54.243 | 50.317 | 14.175 | 1.00 | 34.68 |
| 9703 | O | HOH | X | 161 | 66.368 | 78.182 | -9.856 | 1.00 | 26.10 |
| 9706 | O | HOH | X | 162 | 53.159 | 57.048 | 10.179 | 1.00 | 27.95 |
| 9709 | O | HOH | X | 163 | 44.219 | 16.007 | -6.192 | 1.00 | 25.11 |
| 9712 | O | HOH | X | 164 | 80.589 | 61.008 | 18.291 | 1.00 | 25.88 |
| 9715 | O | HOH | X | 165 | 28.989 | 38.706 | 2.563 | 1.00 | 25.75 |
| 9718 | O | HOH | X | 166 | 11.238 | 30.773 | 0.615 | 1.00 | 24.14 |
| 9721 | O | HOH | X | 167 | 53.608 | 73.127 | 12.234 | 1.00 | 26.24 |
| 9724 | O | HOH | X | 169 | 63.586 | 45.033 | 14.349 | 1.00 | 31.13 |
| 9727 | O | HOH | X | 170 | 77.596 | 48.785 | 23.097 | 1.00 | 26.73 |
| 9730 | O | HOH | X | 171 | 84.848 | 48.026 | 14.304 | 1.00 | 29.46 |
| 9733 | O | HOH | X | 172 | 4.265 | 15.315 | 11.290 | 1.00 | 29.33 |
| 9736 | O | HOH | X | 173 | 3.381 | 31.069 | 16.737 | 1.00 | 33.72 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 9739 | O | HOH | X | 174 | 55.238 | 65.487 | 7.142 | 1.00 | 31.03 |
| 9742 | O | HOH | X | 175 | 9.341 | 26.913 | -11.288 | 1.00 | 29.49 |
| 9745 | O | HOH | X | 176 | 53.199 | 53.483 | 20.584 | 1.00 | 32.49 |
| 9748 | O | HOH | X | 177 | 14.338 | 14.643 | -5.988 | 1.00 | 23.99 |
| 9751 | O | HOH | X | 178 | 38.329 | 22.112 | -11.565 | 1.00 | 45.14 |
| 9754 | O | HOH | X | 179 | 39.337 | 18.256 | 2.081 | 1.00 | 27.57 |
| 9757 | O | HOH | X | 180 | 56.191 | 81.845 | 4.467 | 1.00 | 30.98 |
| 9760 | O | HOH | X | 181 | 20.859 | 16.036 | -15.248 | 1.00 | 24.19 |
| 9763 | O | HOH | X | 182 | 52.592 | 52.636 | 34.412 | 1.00 | 33.36 |
| 9766 | O | HOH | X | 183 | 8.751 | 22.025 | 4.991 | 1.00 | 21.08 |
| 9769 | O | HOH | X | 184 | 63.183 | 88.654 | 8.668 | 1.00 | 32.88 |
| 9772 | O | HOH | X | 185 | 23.296 | 39.123 | 11.088 | 1.00 | 28.53 |
| 9775 | O | HOH | X | 186 | 21.029 | 42.374 | -4.623 | 1.00 | 40.24 |
| 9778 | O | HOH | X | 187 | 61.193 | 73.706 | -5.808 | 1.00 | 35.26 |
| 9781 | O | HOH | X | 188 | 55.468 | 47.798 | 19.949 | 1.00 | 28.75 |
| 9784 | O | HOH | X | 189 | 35.734 | 28.370 | -1.891 | 1.00 | 42.91 |
| 9787 | O | HOH | X | 190 | 28.941 | 9.752 | -9.745 | 1.00 | 28.83 |
| 9790 | O | HOH | X | 191 | 60.836 | 85.243 | -5.478 | 1.00 | 33.63 |
| 9793 | O | HOH | X | 193 | 85.606 | 61.921 | 11.265 | 1.00 | 33.58 |
| 9796 | O | HOH | X | 194 | 78.387 | 74.119 | -1.722 | 1.00 | 50.78 |
| 9799 | O | HOH | X | 195 | 7.183 | 30.679 | 0.916 | 1.00 | 33.15 |
| 9802 | O | HOH | X | 196 | 32.652 | 28.076 | -18.831 | 1.00 | 28.06 |
| 9805 | O | HOH | X | 197 | 53.948 | 51.530 | 21.729 | 1.00 | 30.16 |
| 9808 | O | HOH | X | 198 | 3.740 | 12.442 | 13.203 | 1.00 | 38.10 |
| 9811 | O | HOH | X | 199 | 81.671 | 47.299 | 9.794 | 1.00 | 39.29 |
| 9814 | O | HOH | X | 200 | 76.149 | 46.441 | 21.909 | 1.00 | 32.74 |
| 9817 | O | HOH | X | 201 | 61.151 | 42.663 | 13.748 | 1.00 | 62.81 |
| 9820 | O | HOH | X | 202 | 54.688 | 79.719 | 12.391 | 1.00 | 30.29 |
| 9823 | O | HOH | X | 203 | 51.275 | 79.190 | 10.957 | 1.00 | 40.83 |
| 9826 | O | HOH | X | 204 | 14.506 | 30.823 | -3.503 | 1.00 | 21.42 |
| 9829 | O | HOH | X | 205 | 14.195 | 32.814 | -1.332 | 1.00 | 19.33 |
| 9832 | O | HOH | X | 206 | 12.434 | 31.396 | 3.683 | 1.00 | 16.08 |
| 9835 | O | HOH | X | 207 | 18.969 | 32.213 | 3.765 | 1.00 | 20.53 |
| 9838 | O | HOH | X | 208 | 17.536 | 34.005 | 5.600 | 1.00 | 16.75 |
| 9841 | O | HOH | X | 209 | 33.461 | 39.878 | 0.879 | 1.00 | 48.09 |
| 9844 | O | HOH | X | 210 | 78.263 | 66.876 | 16.527 | 1.00 | 37.29 |
| 9847 | O | HOH | X | 211 | 80.975 | 67.293 | 15.894 | 1.00 | 39.50 |
| 9850 | O | HOH | X | 212 | 82.405 | 67.613 | 13.856 | 1.00 | 46.74 |
| 9853 | O | HOH | X | 213 | 50.671 | 57.527 | 11.069 | 1.00 | 40.42 |
| 9856 | O | HOH | X | 214 | 51.601 | 55.517 | 13.513 | 1.00 | 33.26 |
| 9859 | O | HOH | X | 215 | 62.729 | 54.517 | 30.771 | 1.00 | 40.62 |
| 9862 | O | HOH | X | 216 | 60.331 | 52.329 | 31.300 | 1.00 | 52.01 |
| 9865 | O | HOH | X | 217 | 31.078 | 32.997 | -9.951 | 1.00 | 29.54 |
| 9868 | O | HOH | X | 218 | 33.614 | 33.829 | -1.558 | 1.00 | 23.66 |
| 9871 | O | HOH | X | 219 | 3.882 | 31.855 | 12.746 | 1.00 | 38.99 |
| 9874 | O | HOH | X | 220 | 15.840 | 40.330 | -3.855 | 1.00 | 26.18 |
| 9877 | O | HOH | X | 221 | 15.995 | 38.459 | -6.211 | 1.00 | 24.53 |
| 9880 | O | HOH | X | 222 | 63.555 | 73.039 | -4.552 | 1.00 | 36.76 |
| 9883 | O | HOH | X | 223 | 65.686 | 72.948 | -6.046 | 1.00 | 30.87 |
| 9886 | O | HOH | X | 224 | 61.071 | 89.367 | 2.768 | 1.00 | 33.44 |
| 9889 | O | HOH | X | 225 | 85.368 | 50.306 | 25.290 | 1.00 | 39.68 |
| 9892 | O | HOH | X | 226 | 10.770 | 31.661 | -1.862 | 1.00 | 30.59 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 9895 | O | HOH | X | 227 | 67.074 | 86.090 | 20.611 | 1.00 | 47.90 |
| 9898 | O | HOH | X | 228 | 72.225 | 82.393 | 20.309 | 1.00 | 28.15 |
| 9901 | O | HOH | X | 229 | 23.258 | 30.948 | -19.639 | 1.00 | 37.49 |
| 9904 | O | HOH | X | 230 | 18.514 | 43.214 | -15.138 | 1.00 | 25.15 |
| 9907 | O | HOH | X | 231 | 18.316 | 39.793 | -17.580 | 1.00 | 30.27 |
| 9910 | O | HOH | X | 232 | 18.565 | 40.376 | -20.157 | 1.00 | 27.88 |
| 9913 | O | HOH | X | 233 | 10.124 | 22.994 | 6.965 | 1.00 | 22.65 |
| 9916 | O | HOH | X | 234 | 40.682 | 5.559 | 16.461 | 1.00 | 35.43 |
| 9919 | O | HOH | X | 235 | 60.087 | 44.060 | 7.813 | 1.00 | 29.04 |
| 9922 | O | HOH | X | 236 | 65.753 | 46.800 | 19.256 | 1.00 | 33.55 |
| 9925 | O | HOH | X | 237 | 47.350 | 74.880 | 26.880 | 1.00 | 40.56 |
| 9928 | O | HOH | X | 238 | 48.590 | 70.295 | 28.815 | 1.00 | 22.47 |
| 9931 | O | HOH | X | 239 | 62.111 | 62.571 | -5.691 | 1.00 | 41.29 |
| 9934 | O | HOH | X | 240 | 58.266 | 75.096 | 6.385 | 1.00 | 20.97 |
| 9937 | O | HOH | X | 241 | 57.930 | 77.196 | 8.555 | 1.00 | 21.06 |
| 9940 | O | HOH | X | 242 | 60.766 | 78.814 | 9.905 | 1.00 | 24.54 |
| 9943 | O | HOH | X | 243 | 61.087 | 78.751 | 12.516 | 1.00 | 17.96 |
| 9946 | O | HOH | X | 244 | 66.063 | 45.873 | 5.892 | 1.00 | 30.86 |
| 9949 | O | HOH | X | 245 | 68.834 | 44.595 | 6.140 | 1.00 | 27.12 |
| 9952 | O | HOH | X | 246 | 40.240 | 21.104 | -0.696 | 1.00 | 29.77 |
| 9955 | O | HOH | X | 247 | 54.038 | 67.321 | 16.979 | 1.00 | 23.18 |
| 9958 | O | HOH | X | 248 | 6.161 | 36.828 | -2.610 | 1.00 | 45.75 |
| 9961 | O | HOH | X | 249 | 32.414 | 42.931 | -5.770 | 1.00 | 26.20 |
| 9964 | O | HOH | X | 250 | 8.263 | 18.675 | -2.300 | 1.00 | 37.46 |
| 9967 | O | HOH | X | 251 | 57.682 | 88.576 | 6.524 | 1.00 | 41.67 |
| 9970 | O | HOH | X | 252 | 9.403 | 38.851 | 14.485 | 1.00 | 38.72 |
| 9973 | O | HOH | X | 253 | 7.150 | 40.262 | 16.390 | 1.00 | 45.72 |
| 9976 | O | HOH | X | 254 | 53.657 | 64.735 | -1.870 | 1.00 | 50.87 |
| 9979 | O | HOH | X | 255 | 54.909 | 49.982 | 11.303 | 1.00 | 29.97 |
| 9982 | O | HOH | X | 256 | 54.469 | 48.142 | 15.766 | 1.00 | 35.94 |
| 9985 | O | HOH | X | 257 | 64.819 | 51.877 | 25.591 | 1.00 | 48.64 |
| 9988 | O | HOH | X | 258 | 48.466 | 60.211 | 34.761 | 1.00 | 34.69 |
| 9991 | O | HOH | X | 259 | 50.594 | 60.418 | 33.231 | 1.00 | 29.29 |
| 9994 | O | HOH | X | 260 | 44.303 | 61.380 | 23.666 | 1.00 | 50.60 |
| 9997 | O | HOH | X | 261 | 42.915 | 58.238 | 26.279 | 1.00 | 44.44 |
| 10000 | O | HOH | X | 262 | 52.554 | 63.196 | 6.954 | 1.00 | 45.59 |
| 10003 | O | HOH | X | 263 | 75.789 | 43.073 | 11.027 | 1.00 | 45.52 |
| 10006 | O | HOH | X | 264 | 63.099 | 46.831 | 5.108 | 1.00 | 38.28 |
| 10009 | O | HOH | X | 265 | 44.196 | 64.994 | 15.827 | 1.00 | 37.65 |
| 10012 | O | HOH | X | 266 | 43.951 | 62.363 | 16.102 | 1.00 | 46.48 |
| 10015 | O | HOH | X | 267 | 39.222 | 63.891 | 21.996 | 1.00 | 52.12 |
| 10018 | O | HOH | X | 268 | 42.850 | 63.664 | 23.396 | 1.00 | 50.80 |
| 10021 | O | HOH | X | 269 | 48.526 | 74.293 | 31.675 | 1.00 | 36.34 |
| 10024 | O | HOH | X | 270 | 67.670 | 48.672 | 31.258 | 1.00 | 51.39 |
| 10027 | O | HOH | X | 271 | 81.199 | 48.984 | 16.751 | 1.00 | 28.66 |
| 10030 | O | HOH | X | 272 | 79.911 | 47.943 | 14.775 | 1.00 | 31.46 |
| 10033 | O | HOH | X | 273 | 85.017 | 50.279 | 19.126 | 1.00 | 30.80 |
| 10036 | O | HOH | X | 274 | 64.657 | 81.303 | 10.384 | 1.00 | 30.96 |
| 10039 | O | HOH | X | 275 | 62.329 | 87.607 | 6.341 | 1.00 | 31.55 |
| 10042 | O | HOH | X | 276 | 64.640 | 86.808 | 5.080 | 1.00 | 34.11 |
| 10045 | O | HOH | X | 277 | 60.179 | 93.225 | 8.295 | 1.00 | 40.09 |
| 10048 | O | HOH | X | 278 | 73.593 | 79.168 | 1.381 | 1.00 | 35.41 |

# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 10051 | O | HOH | X | 279 | 74.858 | 77.325 | -0.481 | 1.00 | 41.75 |
| 10054 | O | HOH | X | 280 | 77.068 | 76.446 | 0.836 | 1.00 | 38.59 |
| 10057 | O | HOH | X | 281 | 74.159 | 76.085 | -2.785 | 1.00 | 31.06 |
| 10060 | O | HOH | X | 282 | 79.283 | 78.702 | 16.390 | 1.00 | 38.20 |
| 10063 | O | HOH | X | 283 | 77.257 | 76.993 | 10.420 | 1.00 | 32.78 |
| 10066 | O | HOH | X | 284 | 77.239 | 78.246 | 8.067 | 1.00 | 37.50 |
| 10069 | O | HOH | X | 285 | 73.948 | 68.872 | 7.682 | 1.00 | 33.72 |
| 10072 | O | HOH | X | 286 | 77.608 | 62.256 | 8.543 | 1.00 | 45.53 |
| 10075 | O | HOH | X | 287 | 84.634 | 47.863 | 10.649 | 1.00 | 33.57 |
| 10078 | O | HOH | X | 288 | 89.171 | 59.221 | 10.145 | 1.00 | 51.60 |
| 10081 | O | HOH | X | 289 | 88.540 | 58.568 | 7.606 | 1.00 | 57.77 |
| 10084 | O | HOH | X | 290 | 44.965 | 73.834 | 1.582 | 1.00 | 48.13 |
| 10087 | O | HOH | X | 291 | 49.561 | 81.495 | 7.222 | 1.00 | 45.30 |
| 10090 | O | HOH | X | 292 | 70.469 | 68.660 | -8.004 | 1.00 | 41.08 |
| 10093 | O | HOH | X | 293 | 81.881 | 67.174 | -2.963 | 1.00 | 39.74 |
| 10096 | O | HOH | X | 294 | 77.288 | 57.817 | -5.855 | 1.00 | 32.90 |
| 10099 | O | HOH | X | 295 | 76.204 | 60.286 | -6.405 | 1.00 | 33.62 |
| 10102 | O | HOH | X | 296 | 72.178 | 51.978 | -1.088 | 1.00 | 40.76 |
| 10105 | O | HOH | X | 297 | 69.367 | 55.952 | -6.441 | 1.00 | 41.52 |
| 10108 | O | HOH | X | 298 | 66.145 | 60.092 | -7.585 | 1.00 | 37.64 |
| 10111 | O | HOH | X | 299 | 58.836 | 67.727 | -7.779 | 1.00 | 45.55 |
| 10114 | O | HOH | X | 300 | 13.363 | 3.105 | -5.157 | 1.00 | 38.92 |
| 10117 | O | HOH | X | 301 | 13.794 | 2.664 | -0.805 | 1.00 | 33.87 |
| 10120 | O | HOH | X | 302 | 15.442 | 1.396 | 0.758 | 1.00 | 53.73 |
| 10123 | O | HOH | X | 303 | 17.525 | -0.047 | 0.589 | 1.00 | 35.96 |
| 10126 | O | HOH | X | 304 | 13.277 | 5.297 | -9.056 | 1.00 | 41.07 |
| 10129 | O | HOH | X | 305 | 10.451 | 8.808 | -4.245 | 1.00 | 33.55 |
| 10132 | O | HOH | X | 306 | 11.127 | 5.641 | 1.860 | 1.00 | 28.72 |
| 10135 | O | HOH | X | 307 | 17.465 | 2.139 | -2.799 | 1.00 | 30.54 |
| 10138 | O | HOH | X | 308 | 19.535 | 2.393 | -4.513 | 1.00 | 33.31 |
| 10141 | O | HOH | X | 309 | 9.312 | 12.628 | 0.396 | 1.00 | 37.60 |
| 10144 | O | HOH | X | 310 | 7.665 | 11.510 | 3.549 | 1.00 | 34.31 |
| 10147 | O | HOH | X | 311 | 6.051 | 11.080 | 6.071 | 1.00 | 39.84 |
| 10150 | O | HOH | X | 312 | 10.116 | 7.158 | 11.883 | 1.00 | 33.40 |
| 10153 | O | HOH | X | 313 | 9.385 | 9.324 | 10.796 | 1.00 | 36.05 |
| 10156 | O | HOH | X | 314 | 14.622 | 2.412 | 13.739 | 1.00 | 31.45 |
| 10159 | O | HOH | X | 315 | 13.037 | 2.160 | 16.038 | 1.00 | 41.01 |
| 10162 | O | HOH | X | 316 | 5.930 | 10.969 | 15.786 | 1.00 | 34.44 |
| 10165 | O | HOH | X | 317 | 4.581 | 9.801 | 22.907 | 1.00 | 46.13 |
| 10168 | O | HOH | X | 318 | 1.584 | 18.885 | -1.559 | 1.00 | 52.72 |
| 10171 | O | HOH | X | 319 | 37.184 | 2.115 | -2.954 | 1.00 | 43.48 |
| 10174 | O | HOH | X | 320 | 36.733 | 3.493 | -6.561 | 1.00 | 45.09 |
| 10177 | O | HOH | X | 321 | 20.082 | 0.677 | 4.712 | 1.00 | 26.47 |
| 10180 | O | HOH | X | 322 | 20.457 | 8.134 | 16.042 | 1.00 | 46.78 |
| 10183 | O | HOH | X | 323 | 19.090 | 10.262 | 18.888 | 1.00 | 37.59 |
| 10186 | O | HOH | X | 324 | 24.214 | 25.499 | 12.581 | 1.00 | 29.01 |
| 10189 | O | HOH | X | 325 | 14.989 | 39.048 | 7.973 | 1.00 | 31.76 |
| 10192 | O | HOH | X | 326 | 11.756 | 39.045 | 9.415 | 1.00 | 50.88 |
| 10195 | O | HOH | X | 327 | 7.810 | 36.884 | 3.543 | 1.00 | 43.84 |
| 10198 | O | HOH | X | 328 | 3.242 | 25.497 | -3.703 | 1.00 | 29.56 |
| 10201 | O | HOH | X | 329 | 1.219 | 33.875 | 16.266 | 1.00 | 46.56 |
| 10204 | O | HOH | X | 330 | 1.544 | 29.687 | 13.872 | 1.00 | 40.23 |

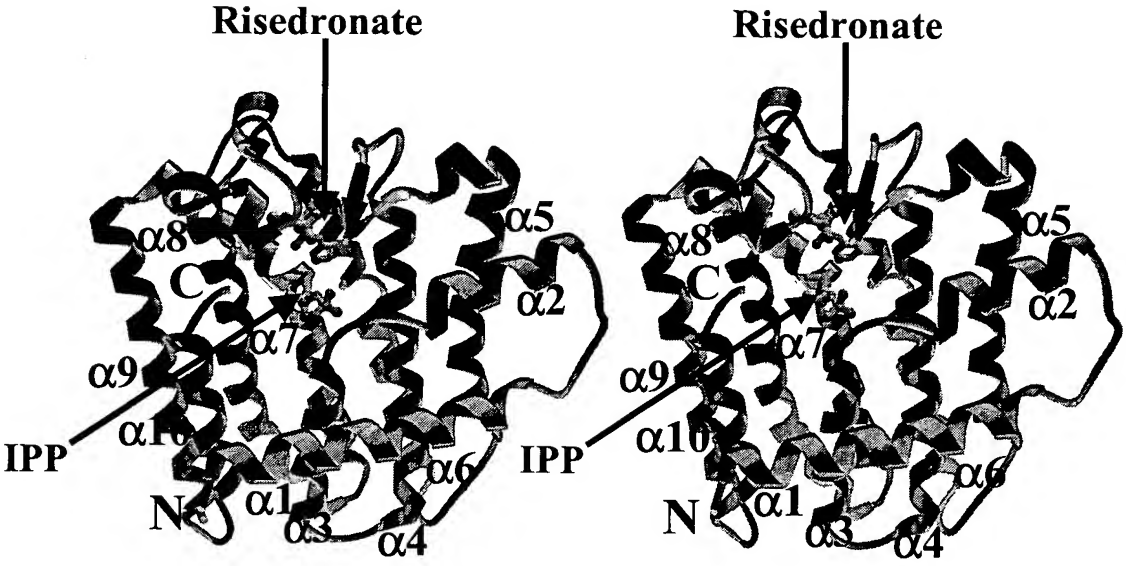
# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 10207 | O | HOH | X | 331 | -0.474 | 27.413 | 15.144 | 1.00 | 54.89 |
| 10210 | O | HOH | X | 332 | 4.337 | 28.953 | 19.199 | 1.00 | 36.94 |
| 10213 | O | HOH | X | 333 | -1.539 | 27.356 | 11.980 | 1.00 | 45.30 |
| 10216 | O | HOH | X | 334 | -2.107 | 24.658 | 12.397 | 1.00 | 38.86 |
| 10219 | O | HOH | X | 335 | 2.398 | 22.547 | 20.759 | 1.00 | 43.49 |
| 10222 | O | HOH | X | 336 | 4.084 | 16.237 | 25.067 | 1.00 | 35.34 |
| 10225 | O | HOH | X | 337 | 3.978 | 13.588 | 25.815 | 1.00 | 45.80 |
| 10228 | O | HOH | X | 338 | 3.094 | 17.271 | 27.390 | 1.00 | 40.72 |
| 10231 | O | HOH | X | 339 | 4.241 | 24.783 | 21.717 | 1.00 | 35.53 |
| 10234 | O | HOH | X | 340 | 37.329 | 4.276 | 7.908 | 1.00 | 35.31 |
| 10237 | O | HOH | X | 341 | 39.684 | 14.815 | 17.121 | 1.00 | 27.65 |
| 10240 | O | HOH | X | 342 | 36.317 | 20.283 | 10.218 | 1.00 | 40.32 |
| 10243 | O | HOH | X | 343 | 32.070 | 22.082 | 3.932 | 1.00 | 19.26 |
| 10246 | O | HOH | X | 344 | 32.703 | 24.069 | 5.500 | 1.00 | 30.65 |
| 10249 | O | HOH | X | 345 | 21.195 | 37.054 | 0.700 | 1.00 | 23.85 |
| 10252 | O | HOH | X | 346 | 26.360 | 48.147 | -1.801 | 1.00 | 37.57 |
| 10255 | O | HOH | X | 347 | 23.190 | 43.465 | -4.592 | 1.00 | 34.90 |
| 10258 | O | HOH | X | 348 | 18.440 | 43.181 | -3.522 | 1.00 | 30.15 |
| 10261 | O | HOH | X | 349 | 15.607 | 42.903 | -4.850 | 1.00 | 31.05 |
| 10264 | O | HOH | X | 350 | 13.692 | 44.194 | -3.391 | 1.00 | 41.66 |
| 10267 | O | HOH | X | 351 | 31.128 | 44.045 | -7.531 | 1.00 | 41.41 |
| 10270 | O | HOH | X | 352 | 31.689 | 47.433 | -4.627 | 1.00 | 30.20 |
| 10273 | O | HOH | X | 353 | 32.993 | 49.163 | -3.190 | 1.00 | 38.18 |
| 10276 | O | HOH | X | 354 | 27.426 | 44.095 | -10.304 | 1.00 | 33.92 |
| 10279 | O | HOH | X | 355 | 43.796 | 13.725 | 3.108 | 1.00 | 23.99 |
| 10282 | O | HOH | X | 356 | 42.070 | 17.335 | 1.525 | 1.00 | 30.43 |
| 10285 | O | HOH | X | 357 | 43.287 | 19.448 | 0.553 | 1.00 | 33.75 |
| 10288 | O | HOH | X | 358 | 39.828 | 16.002 | 5.397 | 1.00 | 35.08 |
| 10291 | O | HOH | X | 359 | 38.165 | 17.818 | 4.577 | 1.00 | 37.82 |
| 10294 | O | HOH | X | 360 | 33.950 | 17.800 | -1.148 | 1.00 | 45.50 |
| 10297 | O | HOH | X | 361 | 11.762 | 24.758 | -4.528 | 1.00 | 31.90 |
| 10300 | O | HOH | X | 362 | 3.975 | 32.061 | -8.760 | 1.00 | 36.38 |
| 10303 | O | HOH | X | 363 | 15.528 | 42.830 | -7.772 | 1.00 | 35.25 |
| 10306 | O | HOH | X | 364 | 14.500 | 29.223 | -15.075 | 1.00 | 41.38 |
| 10309 | O | HOH | X | 365 | 32.850 | 21.982 | -18.707 | 1.00 | 37.44 |
| 10312 | O | HOH | X | 366 | 40.592 | 8.573 | -5.209 | 1.00 | 37.21 |
| 10315 | O | HOH | X | 367 | 25.811 | 11.663 | -16.176 | 1.00 | 30.06 |
| 10318 | O | HOH | X | 368 | 26.945 | 13.028 | -17.719 | 1.00 | 49.20 |
| 10321 | O | HOH | X | 369 | 24.479 | 22.182 | -17.748 | 1.00 | 49.87 |
| 10324 | O | HOH | X | 370 | 21.021 | 17.997 | -19.491 | 1.00 | 46.80 |
| 10327 | O | HOH | X | 371 | 23.217 | 19.367 | -20.360 | 1.00 | 51.32 |
| 10330 | O | HOH | X | 372 | 22.674 | 25.397 | -19.288 | 1.00 | 43.41 |
| 10333 | O | HOH | X | 373 | 12.811 | 20.249 | -12.633 | 1.00 | 35.30 |
| 10336 | O | HOH | X | 374 | 55.709 | 88.998 | 19.001 | 1.00 | 47.10 |
| 10339 | O | HOH | X | 375 | 54.100 | 84.683 | 17.666 | 1.00 | 43.29 |
| 10342 | O | HOH | X | 376 | 48.970 | 77.908 | 17.748 | 1.00 | 39.82 |
| 10345 | O | HOH | X | 377 | 41.899 | 65.707 | 18.118 | 1.00 | 46.67 |
| 10348 | O | HOH | X | 378 | 48.368 | 58.949 | 18.441 | 1.00 | 30.58 |
| 10351 | O | HOH | X | 379 | 48.070 | 56.991 | 22.120 | 1.00 | 35.54 |
| 10354 | O | HOH | X | 380 | 47.998 | 54.800 | 20.225 | 1.00 | 42.38 |
| 10357 | O | HOH | X | 381 | 50.349 | 57.710 | 17.797 | 1.00 | 39.16 |
| 10360 | O | HOH | X | 382 | 32.392 | 26.723 | 0.642 | 1.00 | 35.35 |

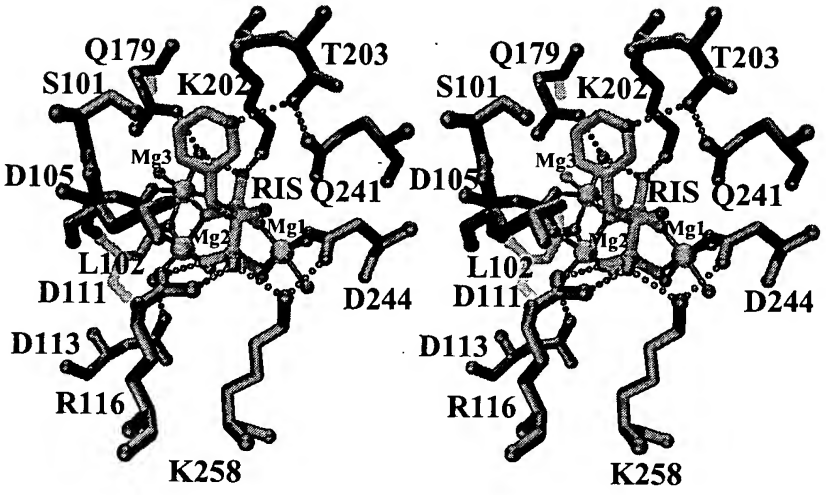
# FIGURE 3 (Cont.)

| A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|
| 10363 | O | HOH | X | 383 | 30.720 | 27.097 | -2.250 | 1.00 | 27.18 |
| 10366 | O | HOH | X | 384 | 37.015 | 26.821 | 2.778 | 1.00 | 49.37 |
| 10369 | O | HOH | X | 385 | 38.443 | 23.443 | 3.534 | 1.00 | 33.87 |
| 10372 | O | HOH | X | 386 | 38.669 | 19.697 | 6.394 | 1.00 | 36.31 |
| 10375 | O | HOH | X | 387 | 30.186 | -3.337 | 5.179 | 1.00 | 43.04 |
| 10378 | O | HOH | X | 388 | 36.379 | 2.179 | 1.556 | 1.00 | 42.15 |
| 10381 | O | HOH | X | 389 | 41.111 | 3.324 | 0.448 | 1.00 | 36.90 |
| 10384 | O | HOH | X | 390 | 43.161 | 2.676 | -1.085 | 1.00 | 38.66 |
| 10387 | O | HOH | X | 391 | 62.047 | 69.399 | 25.389 | 1.00 | 88.66 |
| 10390 | O | HOH | X | 392 | 64.141 | 69.344 | 27.823 | 1.00 | 41.19 |
| 10393 | O | HOH | X | 393 | 58.875 | 89.405 | 12.710 | 1.00 | 64.96 |
| 10396 | O | HOH | X | 394 | 52.351 | 74.162 | -4.548 | 1.00 | 47.29 |
| 10399 | O | HOH | X | 395 | 53.730 | 70.282 | -5.715 | 1.00 | 55.71 |
| 10402 | O | HOH | X | 396 | 47.666 | 76.863 | 1.325 | 1.00 | 34.63 |
| 10405 | O | HOH | X | 397 | 59.660 | 75.843 | -9.785 | 1.00 | 41.09 |
| 10408 | O | HOH | X | 398 | 62.561 | 78.886 | -9.940 | 1.00 | 50.51 |
| 10411 | O | HOH | X | 399 | 30.260 | 2.431 | -11.763 | 1.00 | 34.80 |
| 10414 | O | HOH | X | 400 | 27.528 | 3.971 | -14.875 | 1.00 | 45.91 |
| 10417 | O | HOH | X | 401 | 33.506 | 13.418 | -15.971 | 1.00 | 38.77 |
| 10420 | O | HOH | X | 402 | 41.028 | 6.141 | -7.128 | 1.00 | 49.46 |
| 10423 | O | HOH | X | 403 | 28.710 | 29.035 | -18.837 | 1.00 | 26.44 |
| 10426 | O | HOH | X | 404 | 29.796 | 34.872 | -15.688 | 1.00 | 37.98 |
| 10429 | O | HOH | X | 405 | 27.243 | 36.476 | -15.645 | 1.00 | 37.96 |
| 10432 | O | HOH | X | 406 | 31.047 | 35.920 | -10.224 | 1.00 | 55.58 |
| 10435 | O | HOH | X | 407 | 33.680 | 38.851 | -7.405 | 1.00 | 50.01 |
| 10438 | O | HOH | X | 408 | 25.402 | 37.066 | -19.531 | 1.00 | 37.00 |
| 10441 | O | HOH | X | 409 | 35.153 | 33.776 | 5.764 | 1.00 | 48.02 |
| 10444 | O | HOH | X | 410 | 35.151 | 34.064 | 2.494 | 1.00 | 34.05 |
| 10447 | O | HOH | X | 411 | 34.154 | 30.349 | 7.013 | 1.00 | 44.18 |
| 10450 | O | HOH | X | 412 | 8.762 | 37.486 | 1.397 | 1.00 | 38.43 |
| 10453 | O | HOH | X | 413 | 7.201 | 35.165 | 1.535 | 1.00 | 41.39 |
| 10456 | O | HOH | X | 414 | 26.384 | 40.391 | 4.437 | 1.00 | 36.18 |
| 10459 | O | HOH | X | 415 | 51.309 | 51.810 | -0.301 | 1.00 | 39.62 |
| 10462 | O | HOH | X | 416 | 29.679 | 4.776 | 17.263 | 1.00 | 29.29 |
| 10465 | O | HOH | X | 417 | 28.029 | 5.806 | 20.001 | 1.00 | 42.73 |
| 10468 | O | HOH | X | 418 | 20.603 | 24.902 | 18.280 | 1.00 | 45.48 |
| 10471 | O | HOH | X | 419 | 56.231 | 57.185 | 2.974 | 1.00 | 32.25 |
| 10474 | O | HOH | X | 420 | 53.164 | 57.686 | 5.692 | 1.00 | 35.05 |
| 10477 | O | HOH | X | 421 | 65.428 | 51.862 | 28.325 | 1.00 | 40.33 |

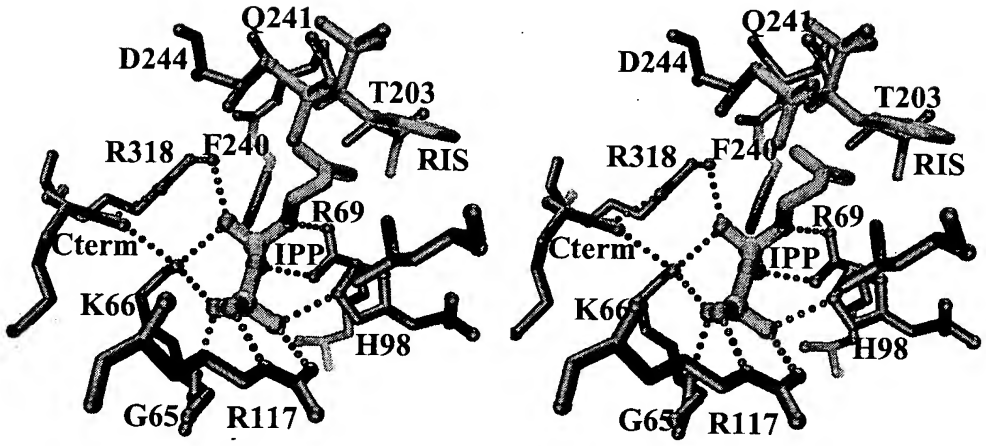
# FIGURE 4


Risedronate
α8
C
α5
α2
α7
α9
IPP
α10
α6
N
α1
α3
α4
Risedronate
α8
C
α5
α2
α7
α9
IPP
α10
α6
N
α1
α3
α4

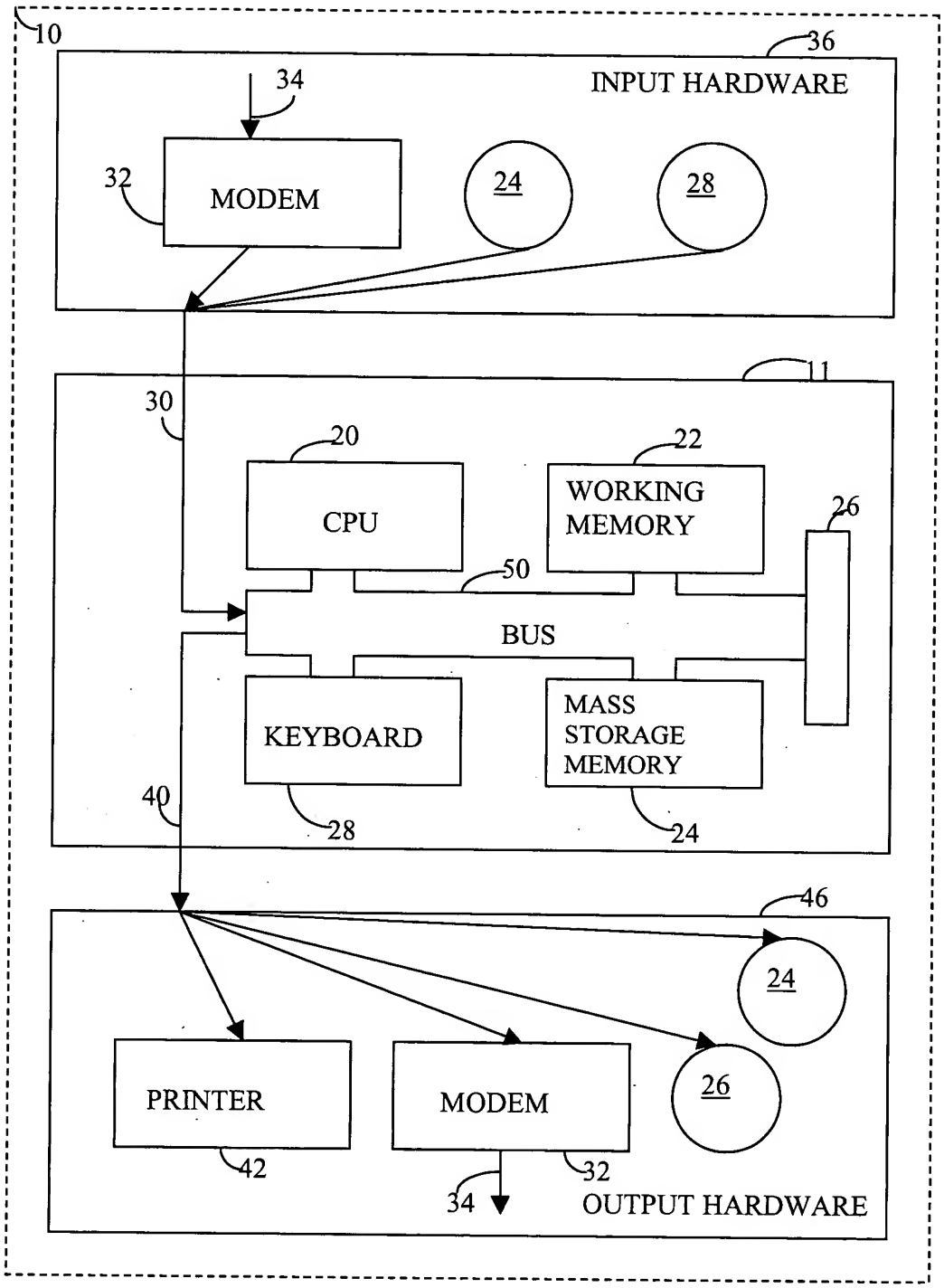
# FIGURE 5A




# FIGURE 5B



# FIGURE 6


10
36
INPUT HARDWARE
34
32
MODEM
24
28
11
30
20
CPU
22
WORKING MEMORY
26
50
BUS
KEYBOARD
MASS STORAGE MEMORY
40
28
24
46
24
PRINTER
MODEM
26
42
32
34
OUTPUT HARDWARE